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(54) Title: DRUG THERAPY FOR CELIAC SPRUE

(57) Abstract: Celiac Sprue and/or dermatitis herpetiformis are treated by interfering with HLA binding of immunogenic gluten peptides. The antigenicity of gluten oligopeptides and the ill effects caused by an immune response thereto are decreased by administration of an HLA-binding peptide inhibitor. Such inhibitors are analogs of immunogenic gluten peptides and (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific T cells.

DRUG THERAPY FOR CELIAC SPRUE

CROSS-REFERENCE TO RELATED APPLICATIONS

This application claims priority to U.S. Provisional Application 60/380,761 filed May 14, 2002; to U.S. Provisional Application 60/392,782 filed June 28, 2002; and to U.S. Provisional application no. 60/422,933, filed October 31, 2002, and to U.S. Provisional Application 60/428,033, filed November 20, 2002, each of which are herein specifically incorporated by reference.

BACKGROUND OF THE INVENTION

In 1953, it was first recognized that ingestion of gluten, a common dietary protein present in wheat, barley and rye causes a disease called Celiac Sprue in sensitive individuals. Gluten is a complex mixture of glutamine- and proline-rich gliadin and glutenin molecules and is thought to be responsible for induction of Celiac Sprue. Ingestion of such proteins by sensitive individuals produces flattening of the normally luxurious, rug-like, epithelial lining of the small intestine known to be responsible for efficient and extensive terminal digestion of peptides and other nutrients. Other clinical symptoms of Celiac Sprue include fatigue, chronic diarrhea, malabsorption of nutrients, weight loss, abdominal distension, anemia, as well as an enhanced risk for the development of osteoporosis and intestinal malignancies such as lymphoma and carcinoma. The disease has an incidence of approximately 1 in 200 in European populations and is believed to be significantly under diagnosed in other populations.

A related disease is dermatitis herpetiformis, which is a chronic eruption of the skin characterized by clusters of intensely pruritic vesicles, papules, and urticaria-like lesions. IgA deposits occur in almost all normal-appearing and perilesional skin. Asymptomatic gluten-sensitive enteropathy is found in 75 to 90% of patients and in some of their relatives. Onset is usually gradual. Itching and burning are severe, and scratching often obscures the primary lesions with eczematization of nearby skin, leading to an erroneous diagnosis of eczema. Strict adherence to a gluten-free diet for prolonged periods may control the disease in some patients, obviating or reducing the requirement for drug therapy. Dapsone, sulfapyridine, and colchicines are sometimes prescribed for relief of itching.

Celiac Sprue (CS) is generally considered to be an autoimmune disease and the antibodies found in the serum of the patients support the theory that the disease is immunological in nature. Antibodies to tissue transglutaminase (TG2, tTGase or tTG) and gliadin appear in almost 100% of the patients with active CS, and the presence of such antibodies, particularly of the IgA class, has been used in diagnosis of the disease.

[05] The large majority of patients express the HLA-DQ2 [DQ(a1*05, b1*02)] and/or DQ8 [DQ(a1*03, b1*0302)] molecules. It is believed that intestinal damage is caused by interactions between specific gliadin oligopeptides and the HLA-DQ2 or DQ8 antigen, which in turn induce proliferation of T lymphocytes in the sub-epithelial layers. T helper 1 cells and cytokines apparently play a major role in a local inflammatory process leading to villous atrophy of the small intestine.

At the present time, there is no good therapy for the disease, except to avoid completely all foods containing gluten. Although gluten withdrawal has transformed the prognosis for children and substantially improved it for adults, some people still die of the disease, mainly adults who had severe disease at the outset. A leading cause of death is lymphoreticular disease, especially intestinal lymphoma. It is not known whether a glutenfree diet diminishes this risk. Apparent clinical remission is often associated with histologic relapse that is detected only by review biopsies or by increased titers of antibodies to tTGase (also called EMA antibodies).

Gluten is so widely used, for example, in commercial soups, sauces, ice creams, hot dogs, and other foodstuffs, that patients need detailed lists of foodstuffs to avoid and expert advice from a dietitian familiar with celiac disease. Ingesting even small amounts of gluten may prevent remission or induce relapse. Supplementary vitamins, minerals, and hematinics may also be required, depending on deficiency. A few patients respond poorly or not at all to gluten withdrawal, either because the diagnosis is incorrect or because the disease is refractory. In the latter case, oral corticosteroids (e.g., prednisone 10 to 20 mg bid) may induce response.

In view of the serious and widespread nature of Celiac Sprue and the difficulty of removing gluten from the diet, better methods of treatment are of great interest. In particular, there is a need for treatment methods that allow the Celiac Sprue individual to eat gluten-containing foodstuffs without ill effect or at least to tolerate such foodstuffs in small or moderate quantities without inducing relapse. The present invention meets this need for better therapies for Celiac Sprue.

SUMMARY OF THE INVENTION

In one aspect, the present invention provides methods for treating Celiac Sprue and/or dermatitis herpetiformis and the symptoms thereof by administration of an HLA-binding peptide inhibitor to the patient. In one embodiment, the HLA-binding peptide inhibitor employed in the method is an analog of an immunogenic gluten peptide, where an immunogenic gluten peptide is altered by the replacement of one or more amino acids, where the replacement may be another naturally occurring amino acid, non-naturally occurring amino acids, modified amino acids, amino acid mimetics, and the like. Analogs of

immunogenic gluten peptides that (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific or other T cells, are useful agents to treat Celiac Sprue.

[10] In another aspect, the present invention provides novel HLA-binding peptide inhibitors and methods for treating Celiac Sprue and/or dermatitis herpetiformis by administering those compounds.

In another aspect, the invention provides pharmaceutical formulations comprising an HLA-binding peptide inhibitor and a pharmaceutically acceptable carrier. In one embodiment, such formulations comprise an enteric coating that allows delivery of the active agent to the intestine, and the agents are stabilized to resist digestion or acid-catalyzed modification in acidic stomach conditions. In another embodiment, the formulation also comprises one or more glutenases, as described in U.S. Provisional Application 60/392,782 filed June 28, 2002; and U.S. Provisional Application 60/428,033, filed November 20, 2002, both of which are incorporated herein by reference. The invention also provides methods for the administration of enteric formulations of one or more HLA-binding peptide inhibitors to treat Celiac Sprue.

In another aspect, the invention provides methods for screening candidate compounds to determine their suitability for use in the subject methods, by assessing the ability of a candidate agent for its ability to bind to HLA molecules, and/or to inhibit the activity of T cells reactive against gluten antigens.

(extracellular) domain of human HLA-DQ2 bound to an immunodominant gluten epitope, and for identifying molecules that will compete with the gluten peptide for MHC binding. In one embodiment, the methods of the invention utilize structural modeling, and the identification and design of molecules having a particular structure. The structural data provided herein is used for the rational design of drugs that affect immune system activation in Celiac Sprue and/or dermatitis herpetiformis. Analysis of the crystal structure in conjunction with sequence data identifies residues in the immunogenic gluten peptide that are important for interaction with the MHC molecule, and those that are accessible for interaction with the T cell antigen receptor. This information provides a basis for rational drug design.

[14] These and other aspects and embodiments of the invention and methods for making and using the invention are described in more detail in the description of the drawings and the invention, the examples, the claims, and the drawings that follow.

DETAILED DESCRIPTION OF THE EMBODIMENTS

Celiac Sprue and/or dermatitis herpetiformis are treated by interfering with HLA binding of immunogenic gluten peptides. Therapeutic benefit can be enhanced in some individuals by increasing the digestion of gluten oligopeptides, whether by pretreatment of foodstuffs to be ingested or by administration of an enzyme capable of digesting the gluten oligopeptides, together with administration of an HLA-binding peptide inhibitor. Gluten oligopeptides are highly resistant to cleavage by gastric and pancreatic peptidases such as pepsin, trypsin, chymotrypsin, and the like, and their prolonged presence in the digestive tract can induce an autoimmune response. The antigenicity of gluten oligopeptides and the ill effects caused by an immune response thereto can be decreased by administration of an HLA-binding peptide inhibitor. Such inhibitors are analogs of immunogenic gluten peptides and (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific or other T cells.

Methods and compositions are provided for the administration of one or more HLA-binding peptide inhibitors to a patient suffering from Celiac Sprue and/or dermatitis herpetiformis. In some embodiments and for some individuals, the methods of the invention remove the requirement that abstention from ingestion of glutens be maintained to keep the disease in remission. The compositions of the invention include formulations of tTGase inhibitors that comprise an enteric coating that allows delivery of the agents to the intestine in an active form; the agents are stabilized to resist digestion or alternative chemical transformations in acidic stomach conditions. In another embodiment, food is pretreated or combined with glutenase, or a glutenase is co-administered (whether in time or in a formulation of the invention) with an HLA-binding peptide inhibitor of the invention.

The subject methods are useful for both prophylactic and therapeutic purposes. Thus, as used herein, the term "treating" is used to refer to both prevention of disease, and treatment of a pre-existing condition. The treatment of ongoing disease, to stabilize or improve the clinical symptoms of the patient, is a particularly important benefit provided by the present invention. Such treatment is desirably performed prior to loss of function in the affected tissues; consequently, the prophylactic therapeutic benefits provided by the invention are also important. Evidence of therapeutic effect may be any diminution in the severity of disease, particularly diminution of the severity of such symptoms as fatigue, chronic diarrhea, malabsorption of nutrients, weight loss, abdominal distension, and anemia. Other disease indicia include the presence of antibodies specific for glutens, antibodies specific for tissue transglutaminase, the presence of pro-inflammatory T cells and cytokines, and degradation of the villus structure of the small intestine. Application of the methods and compositions of the invention can result in the improvement of any and all of these disease indicia of Celiac Sprue.

Patients that can benefit from the present invention include both adults and children. Children in particular benefit from prophylactic treatment, as prevention of early exposure to toxic gluten peptides can prevent development of the disease into its more severe forms. Children suitable for prophylaxis in accordance with the methods of the invention can be identified by genetic testing for predisposition, e.g. by HLA typing; by family history, and by other methods known in the art. As is known in the art for other medications, and in accordance with the teachings herein, dosages of the HLA-binding peptide inhibitors of the invention can be adjusted for pediatric use.

Because most proteases and peptidases are unable to hydrolyze the amide bonds of proline residues, the abundance of proline residues in gliadins and related proteins from wheat, rye and barley can constitute a major digestive obstacle for the enzymes involved. This leads to an increased concentration of relatively stable gluten derived oligopeptides in the gut. These stable gluten derived oligopeptides, called "immunogenic oligopeptides" herein, bind to MHC molecules, including HLA HLA-DQ2 or DQ8 molecules, to stimulate an immune response that results in the autoimmune disease aspects of Celiac Sprue. In some cases the enzyme tissue transglutaminase selectively deamidates certain glutamine residues in these peptides, thereby enhancing their potency for the DQ2 ligand binding pocket.

[20] HLA-binding peptide inhibitors of the present invention are analogs of immunogenic gluten oligopeptides that (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific or other T cells. The inhibitor may comprise oligomers of analogs. Multivalent gluten derived epitopes have markedly enhanced immunogenicity. Consequently, multivalent oligopeptides analogs can also be expected to have increased potency for MHC molecules. In addition, these longer peptides can be more resistant toward intestinal brush border proteolysis.

[21]

An immunogenic gluten oligopeptide analog is an analog of a peptide that comprises at least about 8 residues, and may comprise at least about 10 residues; at least about 11 residues, at least about 12 residues, at least about 13 residues, at least about 14 residues, or more, where the term "residue" refers to naturally occurring amino acids, non-naturally occurring amino acids, and amino acid mimetics or derivatives; and where the gluten peptide is altered by the replacement of one or more amino acids. The replacement may be another naturally occurring amino acid, non-naturally occurring amino acids, modified amino acids, amino acid mimetics, and the like; and may further be derivitized to further reduce the affinity of these ligands for disease-specific T cell receptors. The sequence of immunogenic gluten oligopeptides can be determined by one of skill in the art. Immunogenic gliadin oligopeptides are peptides derived during normal human digestion of gliadins and related storage proteins as described above, from dietary cereals, e.g. wheat, rye, barley, and the

like. Such oligopeptides act as antigens for T cells in Celiac Sprue. For binding to Class II MHC proteins, immunogenic peptides are usually from about 8 to 20 amino acids in length, more usually from about 10 to 18 amino acids. Such peptides may include PXP motifs, such as the motif PQPQLP. Determination of whether an oligopeptide is immunogenic for a particular patient is readily determined by standard T cell activation and other assays known to those of skill in the art.

Among gluten proteins with potential harmful effect to Celiac Sprue patients are [22] included the storage proteins of wheat, species of which include Triticum aestivum; Triticum aethiopicum; Triticum baeoticum; Triticum militinae; Triticum monococcum; Triticum sinskajae; Triticum timopheevii; Triticum turgidum; Triticum urartu, Triticum vavilovii; Triticum zhukovskyi; etc. A review of the genes encoding wheat storage proteins may be found in Colot (1990) Genet Eng (N Y) 12:225-41. Gliadin is the alcohol-soluble protein fraction of wheat gluten. Gliadins are typically rich in glutamine and proline, particularly in the N-terminal part. For example, the first 100 amino acids of α - and γ -gliadins contain ~35% and ~20% of glutamine and proline residues, respectively. Many wheat gliadins have been characterized, and as there are many strains of wheat and other cereals, it is anticipated that many more sequences will be identified using routine methods of molecular biology. Examples of gliadin sequences include but are not limited to wheat alpha gliadin sequences, for example as provided in Genbank, accession numbers AJ133612; AJ133611; AJ133610; AJ133609; AJ133608; AJ133607; AJ133606; AJ133605; AJ133604; AJ133603; AJ133602; D84341.1; U51307; U51306; U51304; U51303; U50984; and U08287. A sequence of wheat omega gliadin is set forth in Genbank accession number AF280605.

Among the immunogenic gluten oligopeptides that may be modified to generate an HLA-binding peptide inhibitor are included the peptide sequence QLQPFPQPELPYP; the sequence PQPELPY; the sequence PFPQPELPYP, PQPELPYPQPQLP, PQQSFPEQQPP, VQGQGIIQPEQPAQ, FPEQPQQPYPQQP, FPQQPEQPYPQQP, FSQPEQEFPQPQ and longer peptides containing such sequences or multiple copies of such sequences. Gliadins, secalins and hordeins contain several PQPQLPY sequences or sequences similar thereto rich in Pro-Gln residues that are high-affinity substrates for tTGase. The tTGase catalyzed deamidation of such sequences increases their affinity for HLA-DQ2, the class II MHC allele present in >90% Celiac Sprue patients. Presentation of these deamidated sequences by DQ2 positive antigen presenting cells effectively stimulates proliferation of gliadin-specific T cells from intestinal biopsies of most Celiac Sprue patients, providing evidence for the proposed mechanism of disease progression in Celiac Sprue.

[24] Analog oligopeptides of the invention comprise at least one difference in amino acid sequence from a native gluten peptide, by the replacement of an amino acid with a different

amino acid; a non-naturally occurring amino acid, a peptidomimetics, substituted amino acid, and the like. An L-amino acid from the native peptide may be altered to any other one of the 20 L-amino acids commonly found in proteins, any one of the corresponding D-amino acids, rare amino acids, such as 4-hydroxyproline, and hydroxylysine, or a non-protein amino acid, such as β-alanine, ornithine and homoserine. Also included with the scope of the present invention are amino acids that have been altered by chemical means such as methylation (e.g., α-methylvaline), deamidation, amidation of the C-terminal amino acid by an alkylamine such as ethylamine, ethanolamine, and ethylene diamine, and acylation or methylation of an amino acid side chain function (e.g., acylation of the epsilon amino group of lysine), deimination of arginine to citrulline, isoaspartylation, or phosphorylation on serine, threonine, tyrosine or histidine residues. Importantly, each of these altered amino acids provide a functional handle, e.g. amine, alcohol, aryl halide, and the like, which can be regioselectively derivatized to further reduce the affinity of these ligands for disease-specific T cell receptors. Peptide analogs may be further derivatized with substitutions, including, without limitation, ethers, amines, esters, amides, carbonates, carbamates, carbazates, ureas and C-C coupled derivatives. Other examples include oxidation of alcohols to ketones, followed by further modifications of the resulting carbonyl group, e.g. via preparation of oximes) or the carbon atom adjacent to the ketone. Such derivatives are encompassed by the term "analog".

The proteolytic stability of gluten oligopeptides can be attributed, at least in part, to the presence of PXP motifs, which are resistant to enzymatic degradation. Preferred analogs of immunogenic gluten oligopeptides will comprise one or more proline residues, and may comprise one or more PXP motifs.

An immunogenic gluten peptide of particular interest is the 33-mer LQLQPFPQPQLPYPQPQLPYPQPQLPYPQPQPP, which is described in detail in International Patent Application US03/04743, herein specifically incorporated by reference. This peptide is both immunogenic and highly stable to proteases. T cell epitopes present in the 33-mer peptide include, *inter alia*, PFPQPQLPY, PQPQLPYPQ, PFPQPELPY; PQPELPYPQ; PYPQPELPY and PYPQPQLPY. In one embodiment of the invention, the immunogenic gluten oligopeptide analog is an analog of a peptide that comprises at least one T cell epitope selected from the group consisting of PFPQPQLPY, PQPQLPYPQ, PFPQPELPY; PQPELPYPQ; PYPQPELPY and PYPQPQLPY.

The structure of an immunogenic gluten oligopeptide bound to a presenting molecule, e.g. HLA-DQ2; HLA-DQ8; etc. can be determined, e.g. by crystallography, NMR, etc., and used to identify residues in a peptide that are involved in the binding to the MHC molecule, and that are involved in the binding to a T cell antigen receptor. Residues identified as accessible for interacting with the T cell receptor may be modified to decrease

the interaction, e.g. by increasing steric hindrance, altering hydrophilicity or hydrophobicity, etc. Residues identified as involved in interaction with the binding cleft of an MHC molecule may be modified to increase the interaction, e.g. by incorporating amino acids known to interact strongly with the binding cleft.

One inhibitor of interest is an oligopeptide or peptidomimetic that comprises the sequence PXPQPELPY, where X is Gly, Ala, Tyr, Trp, Arg, Lys, p-iodo-Phe, 3-iodo-Tyr, p-amino-Phe, 3-amino-Tyr, hydroxylysine, ornithine, Asp, Glu, or any residue that is substantially bulkier or hydrophilic than Phe. Examples of suitable modifications include ethers, amines, esters, amides, carbonates, carbamates, carbazates, ureas and C-C coupled derivatives. Other examples include oxidation of alcohols to ketones, followed by further modifications of the resulting carbonyl group (e.g. via preparation of oximes) or the carbon atom adjacent to the ketone. The peptide may comprise modifications that increase binding potency to an MHC molecule, by varying residues that facilitate peptide docking into the binding cleft. Examples of such residues include Gln-4, Glu-6, Leu-7, and Tyr-9 (numbering based on the epitope PFPQPELPY). Each of these residues interacts closely with several residues in the DQ2 binding pocket. By using structure-based molecular design methods, these interactions can be optimized.

[29] Another inhibitor of interest is a oligopeptide or peptidomimetic that comprises the sequence PFPQX₁ELX₂Y, where X₁ and X₂ are independently selected from 4-hydroxy-Pro (either isomer at C-4), 4-amino-Pro (either isomer atC-4), or 3-hydroxy-Pro (either isomer atC-3), and proline, with the proviso that at least one of X₁ and X₂ is a residue other than proline.

[30] Peptides and peptide analogs may be synthesized by standard chemistry techniques, including synthesis by automated procedure. In general, peptide analogs are prepared by solid-phase peptide synthesis methodology which involves coupling each protected amino acid residue to a resin support, preferably a 4-methylbenzhydrylamine resin, by activation with dicyclohexylcarbodiimide to yield a peptide with a C-terminal amide. Alternatively, a chloromethyl resin (Merrifield resin) may be used to yield a peptide with a free carboxylic acid at the C-terminus. After the last residue has been attached, the protected peptide-resin is treated with hydrogen fluoride to cleave the peptide from the resin, as well as deprotect the side chain functional groups. Crude product can be further purified by gel filtration, HPLC, partition chromatography, or ion-exchange chromatography.

[31] The present invention provides crystals and structures of HLA-DQ2 bound to antigen, where the antigen is an immunogenic gluten peptide QLQPFPQPELPYP, which may be referred to for brevity as an "HLA-DQ2/peptide complex". The structures and structural coordinates are useful in structural homology deduction, and in developing and

screening agents that affect the gluten antigen presentation and immunogenicity. The structure information may be provided in a computer readable form, e.g. as a database of atomic coordinates, or as a three-dimensional model. The structures are useful, for example, in modeling interactions of the HLA molecule with the antigen, effect of inhibitors, etc. The structures are also used to identify molecules that bind to or otherwise interact with structural elements. One aspect of the present invention provides crystals of the HLA-DQ2/peptide complex, which can effectively diffract X-rays for the determination of the atomic coordinates.

The present invention further includes methods of using the structural information provided herein to derive a detailed structure of related peptide binding interactions, particularly other gluten peptides, or analogs and mimetics thereof. Such structural homology determination may utilize modeling, alone or in combination with structure determination.

The present invention provides three-dimensional coordinates for the HLA-DQ2/peptide complex. Such a data set may be provided in computer readable form. Methods of using such coordinates (including in computer readable form) in drug assays and drug screens as exemplified herein, are also part of the present invention. In a particular embodiment of this type, the coordinates contained in the data set can be used to identify potential modulators of the HLA-DQ2/peptide complex, including molecules that mimic the binding of the peptide to the HLA molecule, but which lack, or are substantially diminished in the ability to stimulate a T cell response.

In one embodiment, a potential agent for modulation of HLA-DQ2/peptide complex is selected by performing rational drug design with the three-dimensional coordinates determined for the crystal structures. Preferably the selection is performed in conjunction with computer modeling. Rational design may also be used in the genetic modification of immunogenic peptides by modeling the potential effect of a change in the amino acid sequence.

[35] Computer analysis may be performed with one or more of the computer programs including: GRASP, O (Jones et al. (1991) Acta Cryst. A47:110); QUANTA, CHARMM, INSIGHT, SYBYL, MACROMODEL; ICM, and CNS (Brunger et al. (1998) Acta Cryst. D54:905). In a further embodiment of this aspect of the invention, an initial drug screening assay is performed using the three-dimensional structure so obtained, preferably along with a docking computer program. Such computer modeling can be performed with one or more Docking programs such as DOC, GRAM and AUTO DOCK. See, for example, Dunbrack et al. (1997) Folding & Design 2:27-42.

[36] It should be understood that in the drug screening and protein modification assays provided herein, a number of iterative cycles of any or all of the steps may be performed to

optimize the selection. For example, assays and drug screens that monitor the activity of the T cells in the presence and/or absence of a potential inhibitor are also included in the present invention and can be employed as an assay or drug screen, usually as a single step in a multi-step protocol.

The structure of the HLA-DQ2/peptide complex is useful in the design of agents that mimic the activity and/or specificity of the binding interaction. The structures encoded by the data may be computationally evaluated for an ability to associate with chemical entities. This provides insight into an element's ability to associate with chemical entities. Chemical entities that are capable of associating with these domains may alter immunogenicity. Such chemical entities are potential drug candidates. Alternatively, the structure encoded by the data may be displayed in a graphical format. This allows visual inspection of the structure, as well as visual inspection of the structure's association with chemical entities.

In one embodiment of the invention, an invention is provided for evaluating the ability of a chemical entity to associate with any of the molecules or molecular complexes set forth above. This method comprises the steps of employing computational means to perform a fitting operation between the chemical entity and the interacting surface of the polypeptide or nucleic acid; and analyzing the results of the fitting operation to quantify the association. The term "chemical entity", as used herein, refers to chemical compounds, complexes of at least two chemical compounds, and fragments of such compounds or complexes. Molecular design techniques are used to design and select chemical entities, including inhibitory compounds, capable of binding to the HLA molecule, or to the gluten peptide. Such chemical entities may interact directly with certain key features of the structure.

[39] It will be understood by those skilled in the art that not all of the atoms present in a significant contact residue need be present in a competitive binding agent. In fact, it is only those few atoms that shape the loops and actually form important contacts that are likely to be important for activity. Those skilled in the art will be able to identify these important atoms based on the structure model of the invention, which can be constructed using the structural data herein.

The design of compounds that bind to HLA-DQ2 according to this invention generally involves consideration of two factors. First, the compound must be capable of either competing for binding with an immunogenic gluten peptide; or physically and structurally associating with the HLA-DQ2 domains. Non-covalent molecular interactions important in this association include hydrogen bonding, van der Waals interactions, hydrophobic interactions and electrostatic interactions.

[41] The compound must be able to assume a conformation that allows it to interact with the binding pocket. Although certain portions of the compound will not directly participate in

these associations, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity in relation to all or a portion of the binding pocket, or the spacing between functional groups of an entity comprising several interacting chemical moieties.

Computer-based methods of analysis fall into two broad classes: database methods [42] and de novo design methods. In database methods the compound of interest is compared to all compounds present in a database of chemical structures and compounds whose structure is in some way similar to the compound of interest are identified. The structures in the database are based on either experimental data, generated by NMR or x-ray crystallography, or modeled three-dimensional structures based on two-dimensional data. In de novo design methods, models of compounds whose structure is in some way similar to the compound of interest are generated by a computer program using information derived from known structures, e.g. data generated by x-ray crystallography and/or theoretical rules. Such design methods can build a compound having a desired structure in either an atomby-atom manner or by assembling stored small molecular fragments. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within the interacting surface of the RNA. Docking may be accomplished using software such as Quanta (Molecular Simulations, San Diego, CA) and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

[43] Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include: SmoG, GRID (Goodford (1985) J. Med. Chem., 28, pp. 849-857; Oxford University, Oxford, UK; MCSS (Miranker *et al.* (1991) Proteins: Structure, Function and Genetics, 11, pp. 29-34; Molecular Simulations, San Diego, CA); AUTODOCK (Goodsell *et al.*, (1990) Proteins: Structure, Function, and Genetics, 8, pp. 195-202; Scripps Research Institute, La Jolla, Calif.); and DOCK (Kuntz *et al.* (1982) J. Mol. Biol., 161:269-288; University of California, San Francisco, Calif.)

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or complex. Assembly may be preceded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates. Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include: CAVEAT (Bartlett et al. (1989) In Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 78, pp. 182-196; University of California, Berkeley, Calif.); 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, Calif); and HOOK (available from Molecular Simulations, San Diego, CA).

Other molecular modeling techniques may also be employed in accordance with this invention. See, e.g., N. C. Cohen et al., "Molecular Modeling Software and Methods for Medicinal Chemistry, J. Med. Chem., 33, pp. 883-894 (1990). See also, M. A. Navia et al., "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992).

Once the binding entity has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided. Such substituted chemical compounds may then be analyzed for efficiency of fit by the same computer methods described above.

Another approach made possible and enabled by this invention, is the computational screening of small molecule databases. In this screening, the quality of fit of such entities to the binding site may be judged either by shape complementarity or by estimated interaction energy. Generally the tighter the fit, the lower the steric hindrances, and the greater the attractive forces, the more potent the potential modulator since these properties are consistent with a tighter binding constant. Furthermore, the more specificity in the design of a potential drug the more likely that the drug will not interact as well with other proteins. This will minimize potential side effects due to unwanted interactions with other proteins.

Compounds of interest can be systematically modified by computer modeling programs until one or more promising potential analogs are identified. In addition systematic modification of selected analogs can then be systematically modified by computer modeling programs until one or more potential analogs are identified. Alternatively a potential modulator could be obtained by initially screening a random peptide library, for example one produced by recombinant bacteriophage. A peptide selected in this manner would then be systematically modified by computer modeling programs as described above, and then treated analogously to a structural analog.

Once a potential modulator/inhibitor is identified it can be either selected from a library of chemicals as are commercially available from most large chemical companies including Merck, GlaxoWelcome, Bristol Meyers Squib, Monsanto/Searle, Eli Lilly, Novartis and Pharmacia UpJohn, or alternatively the potential modulator may be synthesized de novo. The de novo synthesis of one or even a relatively small group of specific compounds is reasonable in the art of drug design.

[50] The success of both database and *de novo* methods in identifying compounds with activities similar to the compound of interest depends on the identification of the functionally

relevant portion of the compound of interest. For drugs, the functionally relevant portion may be referred to as a pharmacophore, *i.e.* an arrangement of structural features and functional groups important for biological activity. Not all identified compounds having the desired pharmacophore will act as a modulator of inflammation. The actual activity can be finally determined only by measuring the activity of the compound in relevant biological assays. However, the methods of the invention are extremely valuable because they can be used to greatly reduce the number of compounds that must be tested to identify an actual inhibitor.

In order to determine the biological activity of a candidate pharmacophore it is preferable to measure biological activity at several concentrations of candidate compound. The activity at a given concentration of candidate compound can be tested in a number of ways.

[52] For example, an HLA molecule can be attached to a solid support. Methods for placing proteins on a solid support are well known in the art and include such steps as linking biotin to the protein, and linking avidin to the solid support. The solid support can be washed to remove unreacted species. A solution of a labeled candidate agent can be contacted with the solid support. The solid support is washed again to remove the potential modulator not bound to the support. The amount of labeled potential modulator remaining with the solid support and thereby bound to the protein can be determined. Alternatively, or in addition, the dissociation constant between the labeled candidate agent and the protein can be determined.

Crystals of the binding complex of the present invention can be grown by a number of techniques including batch crystallization, vapor diffusion (either by sitting drop or hanging drop) and by microdialysis. Seeding of the crystals in some instances is required to obtain X-ray quality crystals. Standard micro and/or macro seeding of crystals may therefore be used. The crystals may be shrunk by transfer into solutions of different composition, e.g. by the addition of metal ions such as Mn²⁺, Pb²⁺, etc. Crystals may also be generated that include cofactors, substrates, candidate inhibitors, and the like, that interact with the protein, e.g. by cocrystallization of soaking protein crystals in a solution comprising an inhibitor or other agent.

[54] Alternative methods may also be used. For example, crystals can be characterized by using X-rays produced in a conventional source (such as a sealed tube or a rotating anode) or using a synchrotron source. Methods of characterization include, but are not limited to, precision photography, oscillation photography and diffractometer data collection. Selenium-methionine may be used as described in the examples provided herein, or alternatively a heavy metal derivative data set (e.g., using PCMB) may be used in place of the selenium-methionine derivatization.

[55] Electron density maps may be built from crystals using phase information from multiple isomorphous heavy-atom derivatives, molecular replacement or selenomethionine incorporated multiwavelength anomalous disperson technique. Model building is facilitated by the use of sequence markers, especially selenomethionine residues. Anomalous difference Fourier maps may be calculated with data from selenomethionine-substituted HLA-DQ2/ GLUTEN EPITOPE and with experimental multiple isomorphous replacement with anomalous scattering (MIRAS) phases (Hemming and Edwards (2000) J. Biol. Chem. 275:2288). Maps are improved by phase combination, where MIRAS phases are combined by the program SIGMAA (Jones et al., supra.) Phase combination may be followed by solvent flattening with DM (Carson (1997) Methods Enzymol. 277:493). Improved maps may be obtained by combination of the MIRAS phases with improved phases from combined polyalanine and atomic models in an iterative process. The model can be refined by classical positional and B-factor minimization, and with manual rebuilding.

HLA-DQ2/peptide complex structure models and databases of structure information are provided. The structural models find use in determining the structure of related and/or analogous peptide complexes. In some cases, modeling will be based on the provided structure. In other embodiments, modeling will utilize the provided structure in combination with features present in homologous and/or related structures, where relationship may be defined by protein sequence similarity, or structural similarity, e.g. in the presence of specific features as described above.

[56]

The structure model may be implemented in hardware or software, or a combination of both. For most purposes, in order to use the structure coordinates generated for the structure, it is necessary to convert them into a three-dimensional shape. This is achieved through the use of free or commercially available software that is capable of generating three-dimensional graphical representations of molecules or portions thereof from a set of structure coordinates.

In one embodiment of the invention, a machine-readable storage medium is provided, the medium comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of any of the structures of this invention that have been described above. Specifically, the computer-readable storage medium is capable of displaying a graphical three-dimensional representation of the HLA-DQ2/peptide complex.

[59] Thus, in accordance with the present invention, data providing structural coordinates, alone or in combination with software capable of displaying the resulting three dimensional structure of the complex, portions thereof, and their structurally similar analogs, is stored in a machine-readable storage medium. Such data may be used for a variety of

purposes, such as drug discovery, analysis of interactions between cellular components during translation, modeling of vaccines, and the like.

Preferably, the invention is implemented in computer programs executing on programmable computers, comprising a processor, a data storage system (including volatile and non-volatile memory and/or storage elements), at least one input device, and at least one output device. Program code is applied to input data to perform the functions described above and generate output information. The output information is applied to one or more output devices, in known fashion. The computer may be, for example, a personal computer, microcomputer, or workstation of conventional design.

[61] Each program is preferably implemented in a high level procedural or object oriented programming language to communicate with a computer system. However, the programs can be implemented in assembly or machine language, if desired. In any case, the language may be a compiled or interpreted language.

[62] Each such computer program is preferably stored on a storage media or device (e.g., ROM or magnetic diskette) readable by a general or special purpose programmable computer, for configuring and operating the computer when the storage media or device is read by the computer to perform the procedures described herein. The system may also be considered to be implemented as a computer-readable storage medium, configured with a computer program, where the storage medium so configured causes a computer to operate in a specific and predefined manner to perform the functions described herein.

The HLA-binding peptide inhibitors are incorporated into a variety of formulations for therapeutic administration. In one aspect, the agents are formulated into pharmaceutical compositions by combination with appropriate, pharmaceutically acceptable carriers or diluents, and may be formulated into preparations in solid, semi-solid, liquid or gaseous forms, such as tablets, capsules, powders, granules, ointments, solutions, suppositories, injections, inhalants, gels, microspheres, and aerosols. As such, administration can be achieved in various ways, usually by oral administration. The HLA-binding peptide inhibitors may be systemic after administration or may be localized by virtue of the formulation, or by the use of an implant that acts to retain the active dose at the site of implantation.

In pharmaceutical dosage forms, the HLA-binding peptide inhibitors may be administered in the form of their pharmaceutically acceptable salts, or they may also be used alone or in appropriate association, as well as in combination with other pharmaceutically active compounds. The agents may be combined, as previously described, to provide a cocktail of activities. The following methods and excipients are merely exemplary and are in no way limiting.

[65] For oral preparations, the agents can be used alone or in combination with appropriate additives to make tablets, powders, granules or capsules, for example, with conventional additives, such as lactose, mannitol, corn starch or potato starch; with binders, such as crystalline cellulose, cellulose derivatives, acacia, com starch or gelatins; with disintegrators, such as corn starch, potato starch or sodium carboxymethylcellulose; with lubricants, such as talc or magnesium stearate; and if desired, with diluents, buffering agents, moistening agents, preservatives and flavoring agents.

In one embodiment of the invention, the oral formulations comprise enteric coatings, so that the active agent is delivered to the intestinal tract. Enteric formulations are often used to protect an active ingredient from the strongly acid contents of the stomach. Such formulations are created by coating a solid dosage form with a film of a polymer that is insoluble in acid environments, and soluble in basic environments. Exemplary films are cellulose acetate phthalate, polyvinyl acetate phthalate, hydroxypropyl methylcellulose phthalate and hydroxypropyl methylcellulose acetate succinate, methacrylate copolymers, and cellulose acetate phthalate.

Other enteric formulation comprise engineered polymer microspheres made of biologically erodable polymers, which display strong adhesive interactions with gastrointestinal mucus and cellular linings, can traverse both the mucosal absorptive epithelium and the follicle-associated epithelium covering the lymphoid tissue of Peyer's patches. The polymers maintain contact with intestinal epithelium for extended periods of time and actually penetrate it, through and between cells. See, for example, Mathiowitz et al. (1997) Nature 386 (6623): 410-414. Drug delivery systems can also utilize a core of superporous hydrogels (SPH) and SPH composite (SPHC), as described by Dorkoosh et al. (2001) J Control Release 71(3):307-18.

[68] Formulations are typically provided in a unit dosage form, where the term "unit dosage form," refers to physically discrete units suitable as unitary dosages for human subjects, each unit containing a predetermined quantity of glutenase calculated in an amount sufficient to produce the desired effect in association with a pharmaceutically acceptable diluent, carrier or vehicle. The specifications for the unit dosage forms of the present invention depend on the particular complex employed and the effect to be achieved, and the pharmacodynamics associated with each complex in the host.

The pharmaceutically acceptable excipients, such as vehicles, adjuvants, carriers or diluents, are readily available to the public. Moreover, pharmaceutically acceptable auxiliary substances, such as pH adjusting and buffering agents, tonicity adjusting agents, stabilizers, wetting agents and the like, are readily available to the public.

METHODS OF TREATMENT

The subject methods are used to treat individuals suffering from Celiac Sprue and/or dermatitis herpetiformis, by administering an effective dose through a pharmaceutical formulation. Diagnosis of suitable patients may utilize a variety of criteria known to those of skill in the art. A quantitative increase in antibodies specific for gliadin, and/or tissue transglutaminase is indicative of the disease. Family histories and the presence of the HLA alleles HLA-DQ2 [DQ(a1*05, b1*02)] and/or DQ8 [DQ(a1*03, b1*0302)] are indicative of a susceptibility to the disease. Specific peptide analogs may be administered therapeutically to decrease inflammation, and/or to induce antigen-specific tolerance to treat autoimmunity. Methods for the delivery of peptides that are altered from a native peptide are known in the art. Alteration of native peptides with selective changes of crucial residues can induce unresponsiveness or change the responsiveness of antigen-specific autoreactive T cells.

[71] The therapeutic effect may be measured in terms of clinical outcome, or may rely on immunological or biochemical tests. Suppression of the deleterious T-cell activity can be measured by enumeration of reactive Th1 cells, by quantitating the release of cytokines at the sites of lesions, or using other assays for the presence of autoimmune T cells known in the art. Alternatively, one may look for a reduction in symptoms of a disease.

Various methods for administration may be employed. The dosage of the therapeutic formulation will vary widely, depending upon the nature of the disease, the frequency of administration, the manner of administration, the clearance of the agent from the host, and the like. Such treatment could either be before meals or on a once-a-day basis or on a once-a-week basis, depending on the half-life of the inhibitor. A typical dose is at least about 1 μg, usually at least about 10 μg, more usually at least about 0.1 mg, and not more than about 10 mg, usually not more than about 1 mg. Enteric coating of these peptides may also enhance their lifetimes in the gut, thereby permitting delivery to the proximal and distal small intestinal tissue. Treatment of other autoimmune disorders such as Type I diabetes with such ligands may involve oral, intravenous or intramuscular administration. The initial dose may be larger, followed by smaller maintenance doses. The dose may be administered as infrequently as weekly or biweekly, or more often fractionated into smaller doses and administered daily, with meals, semi-weekly, etc. to maintain an effective dosage level.

The HLA-binding peptide inhibitors of the invention may be administered in the treatment of Type 1 diabetes (IDDM). IDDM and celiac disease are both immunologic disorders where specific HLA alleles are associated with disease risk. Transglutaminase autoantibodies can be found in some patients with IDDM. The prevalence of transglutaminase autoantibodies is higher in diabetic patients with HLA DQ2 or DQ8.

Human type I or insulin-dependent diabetes mellitus (IDDM) is characterized by autoimmune destruction of the β cells in the pancreatic islets of Langerhans. The depletion of β cells results in an inability to regulate levels of glucose in the blood. Overt diabetes occurs when the level of glucose in the blood rises above a specific level, usually about 250 mg/dl. In humans a long presymptomatic period precedes the onset of diabetes. During this period there is a gradual loss of pancreatic beta cell function. IDDM is currently treated by monitoring blood glucose levels to guide injection, or pump-based delivery, of recombinant insulin. Diet and exercise regimens contribute to achieving adequate blood glucose control. The inhibitors of the invention may be administered alone, or in combination with other therapies. The route of administration may be oral, as described for treatment of Celiac Sprue, or may be injected, e.g. i.v., i.m., etc. Administration may be performed during the pre-symptomatic phase, or in overt diabetes.

EXPERIMENTAL

Example

It has long been known that the principal toxic components of wheat gluten are a [75] family of closely related Pro-Gln rich proteins called gliadins. Recent reports have suggested that peptides from a short segment of α-gliadin appear to account for most of the gluten-specific recognition by CD4+ T cells from Celiac Sprue patients. These peptides are substrates of tissue transglutaminase (tTGase), the primary auto-antigen in Celiac Sprue, and the products of this enzymatic reaction bind to the class II HLA DQ2 molecule. This "immunodominant" region of α -gliadin is part of an unusually long proteolytic product generated by the digestive process that: (a) is exceptionally resistant to further breakdown by gastric, pancreatic and intestinal brush border proteases; (b) is the highest specificity substrate of human tissue transglutaminase (tTGase) discovered to date; (c) contains at least six overlapping copies of epitopes known to be recognized by patient derived T cells; (d) stimulates representative T cell clones that recognize these epitopes with submicromolar efficacy; and (e) has homologs in proteins from all toxic foodgrains but no homologs in non-toxic foodgrain proteins.

Identification of stable peptides from gastric protease, pancreatic protease and brush border membrane peptidase catalyzed digestion of recombinant α2-gliadin: α2-gliadin, a representative α-gliadin (Arentz-Hansen et al. (2000) Gut 46:46), was expressed in recombinant form and purified from E. coli. The α2-gliadin gene was cloned in pET28a plasmid (Novagen) and transformed into the expression host BL21(DE3) (Novagen). The transformed cells were grown in 1-liter cultures of LB media containing 50 μg/ml of

kanamycin at 37 $^{\circ}$ C until the OD600 0.6-1 was achieved. The expression of α 2-gliadin protein was induced with the addition of 0.4 mM isopropyl α-D-thiogalactoside (Sigma) and the cultures were further incubated at 37 °C for 20 hours. The cells expressing the recombinant α2-gliadin were centrifuged at 3600 rpm for 30 minutes. The pellet was resuspended in 15 ml of disruption buffer (200 mM sodium phosphate; 200 mM NaCl; 2.5 mM DTT; 1.5 mM benzamidine; 2.5 mM EDTA; 2 mg/L pepstatin; 2 mg/L leupeptin; 30% v/v glycerol) and lysed by sonication (1 minute; output control set to 6). After centrifugation at 45000g for 45 min, the supernatant was discarded and the pellet containing gliadin protein was resuspended in 50 ml of 7M urea in 50 mM Tris (pH = 8.0). The suspension was again centrifuged at 45000g for 45 min and the supernatant was harvested for purification. The supernatant containing α2-gliadin was incubated with 1 ml of nickel-nitrilotriacetic acid resin (Ni-NTA; Qiagen) overnight and then batch-loaded on a column with 2 ml of Ni-NTA. The column was washed with 7M urea in 50 mM Tris (pH = 8.0) and α 2-gliadin was eluted with 200 mM imidazole, 7 M urea in 50 mM Tris (pH = 4.5). The fractions containing α 2-gliadin were pooled into a final concentration of 70% ethanol solution and two volumes of 1.5M NaCl were added to precipitate the protein. The solution was incubated at 4 °C overnight and the final precipitate was collected by centrifugation at 45000 g for 30 min. rinsed in water, and re-centrifuged to remove the urea. The final purification step of the α-2 gliadin was developed with reverse-phase HPLC. The Ni-NTA purified protein fractions were pooled in 7 M urea buffer and injected to a Vydac (Hesperia, CA) polystyrene reversephase column (i.d. 4.6 mm × 25 cm) with the starting solvent (30% of solvent B: 1:1 HPLCgrade acetonitrile/isopropanol: 0.1% TFA). Solvent A was an aqueous solution with 0.1% TFA. The separation gradient extended from 30-100% of solvent B over 120 min at a flow rate of 0.8 ml/min.

Table 2, Amount of Peptides Digested after 15 hours

	33-mer	Control A	Control B
H1P0	<20%	>90%	>90%
H2P0	<20%	>61%	>85%
H3P0	<20%	>87%	>95%
H4P0	<20%	>96%	>95%
H5P0	<20%	>96%	>95%

The purity of the recombinant gliadin was >95%, which allowed for facile identification and assignment of proteolytic products by LC-MS/MS/UV. Although many previous studies utilized pepsin/trypsin treated gliadins, it was found that, among gastric and pancreatic proteases, chymotrypsin played a major role in the breakdown of α2-gliadin,

To establish the physiological relevance of this peptide, composite gastric/pancreatic enzymatic digestion of α2 gliadin was then examined. As expected, enzymatic digestion with pepsin (1:100 w/w ratio), trypsin (1:100), chymotrypsin (1:100), elastase (1:500) and carboxypeptidase (1:100) was quite efficient, leaving behind only a few peptides longer than 9 residues (the minimum size for a peptide to show class II MHC mediated antigenicity). In addition to the above-mentioned 33-mer, the peptide WQIPEQSR was also identified, and was used as a control in many of the following studies.

[79]

The small intestinal brush-border membrane (BBM) enzymes are known to be vital for breaking down any remaining peptides from gastric/pancreatic digestion into amino acids, dipeptides or tripeptides for nutritional uptake. Therefore a comprehensive analysis of gliadin metabolism also required investigations into BBM processing of gliadin peptides of reasonable length derived from gastric and pancreatic protease treatment. BBM fractions were prepared from rat small intestinal mucosa. The specific activities of known BBM peptidases were verified to be within the previously reported range. Whereas the half-life of disappearance of WQIPEQSR was ~60 min in the presence of 12 ng/µl BBM protein, the half-life of LQLQPFPQPQLPYPQPQLPYPQPQLPYPQPQPPQPQF digestion was >20 h. Therefore, the latter peptide remains intact throughout the digestive process in the stomach and upper small intestine, and is poised to act as a potential antigen for T cell proliferation and intestinal toxicity in genetically susceptible individuals.

Example 2

The 33-mer gliadin peptide is an excellent substrate for tTGase, and the resulting product is a highly potent activator of patient-derived T cells: A number of recent studies have demonstrated that regiospecific deamidation of immunogenic gliadin peptides by tTGase increases their affinity for HLA-DQ2 as well as the potency with which they activate patient-derived gluten-specific T cells. It has been shown the specificity of tTGase for certain short antigenic peptides derived from gliadin is higher than its specificity toward its physiological target site in fibronectin, for example, the specificity of tTGase for the α -gliadin

Structural characteristics of the 33-mer gliadin peptide and its naturally occurring [81] homologs: Sequence alignment searches using BLASTP in all non-redundant protein databases revealed several homologs (E-value < 0.001) of the 33-mer gliadin peptide. Interestingly, foodgrain derived homologs were only found in gliadins (from wheat), hordeins (from barley) and secalins (from rye), all of which have been proven to be toxic to Celiac patients (Figure 7). Nontoxic foodgrain proteins, such as avenins (in oats), rice and maize, do not contain homologous sequences to the 33-mer gliadin. In contrast, a BLASTP search with the entire α2-gliadin sequence identified foodgrain protein homologs from both toxic and nontoxic proteins. Based on available information regarding the substrate specificities of gastric, pancreatic and BBM proteases and peptidases, it is predicted that, although most gluten homologs to the 33-mer gliadin peptide contained multiple proteolytic sites and are therefore unlikely to be completely stable toward digestion, several sequences from wheat, rye and barley are expected to be comparably resistant to gastric and intestinal proteolysis. The stable peptide homologs to the 33-mer α2-gliadin peptide are OPQPFPPQLPYPQTQPFPPQQPYPQPQPQPQPQ (from α 1- and α 6-gliadins); QQQPFPQQPIPQQPQPYPQQPQPYPQQPFPPQQPF (from B1 hordein); QPFPQPQQTFPQQPQLPFPQQPQQPFPQPQ (from y-gliadin); VQWPQQQPVPQPHQPF (from γ -gliadin), VQGQGIIQPQQPAQ (from γ -gliadin), FLQPQQPFPQQPQQPYPQQPQQPFPQ (from γ-gliadin), FSQPQQQFPQPQQPQQSFPQQQPP (from γ-gliadin), OPFPQPQQPTPIQPQQPFPQRPQQPFPQPQ (from ω-secalin). These stable peptides are all located at the N-terminal region of the corresponding proteins. The presence of proline residues after otherwise cleavable residues in these peptides would contribute to their proteolytic stability.

The unique primary sequence of the 33-mer gliadin peptide also had homologs among a few non-gluten proteins. Among the strongest homologs were internal sequences from pertactin (a highly immunogenic protein from *Bordetella pertussis*) and a mammalian inositol-polyphosphate 5-phosphatase of unknown function. In both cases available information suggested that the homology could have biologically relevance. For example, the region of pertactin that is homologous to the 33-mer gliadin peptide is known to be part of the immunodominant segment of the protein. In the case of the homologous phosphatase, the corresponding peptide region of the phosphatase is known to be responsible for vesicular trafficking of the phosphatase to the cytoplasmic Golgi. In analogy with the current picture of how gliadin peptides are presented to HLA-DQ2 via a tTGase mediated pathway, these Pro-Gln-rich segments of both pertactin and the phosphatase are likely to be good tTGase substrates.

Example 3

[83] X-ray Crystallographic Analysis of soluble HLA-DQ2. The soluble extracellular domains of the α - and β -chains of HLA-DQ2 were co-expressed in insect cells using a baculovirus expression system (pAcAB3 vector, BD Biosciences). The DNA sequence of the engineered α - and β -chains is provided in SEQ ID NO:1 and SEQ ID NO:2. The β -chain is fused to a sequence encoding the epitope QLQPFPQPELPY at its N-terminal end, and to a biotin recognition sequence at its C-terminal end. Both subunits are also fused to complementary leucine zipper sequences at their C-terminal ends. Since a Factor Xa proteolysis site is engineered between the leucine zipper sequences and the DQ2 subunits, prior to crystallization the leucine zippers were removed from DQ2 by Factor Xa digestion.

[84]

Initial purification of the DQ2 heterodimer from the culture medium was performed on an immunoaffinity column containing an anti-DQ2 monoclonal antibody (2.12.E11) bound to a Protein A Sepharose CL-4B column. Subsequently DQ2 was treated with Factor Xa, and purified from the digestion mixture by anion-exchange chromatography followed by size-exclusion chromatography, and concentrated to 4 mg/ml in 25 mM Tris-HCl, pH 8.0. Crystals of the DQ2-epitope complex were obtained using the hanging drop method. Typically, 2 μL of protein solution (2~4 mg/ml DQ2, 25 mM Tris-HCl, pH 8.0) and 2 μL of precipitant buffer (200 mM ammonium acetate, 40 mM ammonium sulfate, 4% ethylene glycol, 22~26% PEG 3350) were combined in a single drop hanging over 1 mL of precipitant buffer at room temperature. Small crystals appeared within three days and grew to full size in two weeks.

[85] For data collection, crystals were transferred to a cryoprotectant solution (mother liquor containing 28% ethylene glycol) for 2 hours, and then flash cooled at 100K in liquid nitrogen. X-ray diffraction data were collected from a single crystal to 2.22 Å resolution at

beamline 11-1 of the Stanford Synchrotron Radiation Laboratory using a Quantum 315 CCD detector. Oscillation images were processed with DENZO and data reduction was carried out with SCALEPACK.

The structure of DQ2-epitope complex was determined by molecular replacement using the program AMoRe in the CCP4 suite of programs. The 2.4 Å resolution structure of insulin peptide-HLA-DQ8 complex (RCSB accession code: 1JK8) minus the insulin peptide and solvent molecules was used as the search model. After initial refinement with the maximum likelihood function of program REFMAC, iterative cycles of refinement including simulated annealing, temperature factor refinement, and energy minimization were made with the program CNS. Model building and correction were performed using σ_A -weighted F_o - F_c and $2F_o$ - F_c electron density maps with the program O. The current model has R-factor of 0.2209 with a R_{free} of 0.2793 at 2.22 Å resolution. Analysis of the Ramachandran plot generated using the program PROCHECK shows that 91.2 % of residues are in most favored regions, 7.9 % are in additional allowed regions, 0.5 % are in generously allowed regions, and 0.5 % are in disallowed regions.

[87] There are two molecules of DQ2-epitope in the asymmetric unit. In the first complex, α-chain of DQ2, β-chain of DQ2, and the alpha-I epitope peptide (sequence QLQPFPQPELPY) are designated A, B, and C respectively. In the second complex, α-chain, β-chain, and epitope peptide are designated D, E, and F respectively. The model includes 354 water molecules (name: HOH) and 4 ethylene glycol molecules (name: EDO).

Thr-106—His-112 region in chain B and Arg-105—His-112 region in chain E are disordered and thus absent from the model. Superposition of the DQ8 structure suggests that these regions form an extended loop. Side chain conformation of the following residues are undefined due to weak electron density in the corresponding region and therefore only their backbone atoms are included in the model: Asp-135 (in chain B), Leu-2, Gln-3, Tyr-12 (in chain C), Asp-135, Gln-136 (in chain E), and Leu-2, Gln-3 (in chain F).

[89] Structure-based design of DQ2 binding peptide inhibitors. The crystal structure of the DQ2-epitope complex reveals precisely which atoms in the peptide QLQPFPQPELPYP point outward (by inference into the T cell receptor binding pocket). Substitutions at these atoms can yield altered peptide ligands that retain the ability to bind tightly to DQ2 but are no longer able to allow docking of the DQ2-peptide complex into disease specific T cell receptors.

The coordinate of the structure are as follows:

[88]

[90]

Coordinates

REMARK peptide link removed (applied DPEP): from B 105 to B 113 REMARK peptide link removed (applied DPEP): from E 113 104 to B 163 107 REMARK disulphide added: from A to A REMARK disulphide added: from B 15 to B 79 REMARK disulphide added: from B 117 to B 173

REMARK	disulp	hide	add	ed:	from	D	107	to D	163		
REMARK							15	to E	79		
REMARK							117	to E	173		
REMARK REMARK		-		13	3:00:0)6	C	reated by	y user:	kim	
MOTA	1		VAL :		2		31.060	3.851	4.095	1.00 39.43	A
ATOM	2		VAL .		2		30.078	2.835	3.531	1.00 40.06	A
ATOM	3		VAL .		2		30.370	5.185	4.344	1.00 39.97	A
ATOM	4	C	VAL .		2		30.653	3.406	6.542	1.00 36.80	A
MOTA	5	0	VAL .		2		29.644	2.702	6.527 5.235	1.00 38.25 1.00 36.80	A A
MOTA MOTA	6 7	N CA	VAL .		2 2		32.189 31.684	1.926 3.321	5.414	1.00 37.95	A
MOTA	8	N N	ALA		3		30.910	4.267	7.523	1.00 34.99	A
MOTA	9	CA	ALA		3		30.003	4.416	8.658	1.00 32.94	A
MOTA	10	СВ	ALA		3		30.325	3.368	9.721	1.00 33.34	A
MOTA	11	C	ALA	A	3		30.094	5.805	9.263	1.00 30.81	A
MOTA	12	0	ALA		3		30.980	6.583	8.914	1.00 29.57	A
MOTA	13	N	ASP		4		29.172	6.115	10.170	1.00 28.70	A
MOTA	14	CA	ASP		4		29.173	7.416	10.822	1.00 26.95	A
ATOM	15	CB	ASP		4		27.812	7.722	11.456	1.00 28.65	A
MOTA	16	CG	ASP		4		26.687 26.904	7.845 8.417	9.339	1.00 31.67 1.00 33.31	A A
MOTA MOTA	17 18		asp asp		4		25.568	7.381	10.735	1.00 33.31	A
ATOM	19	C	ASP		4		30.254	7.432	11.898	1.00 26.51	A
ATOM	20	ō	ASP		4		30.857	8.469	12.170	1.00 25.25	A
ATOM	21	N	HIS		5		30.493	6.277	12.515	1.00 26.22	A
ATOM	22	CA	HIS	A	5		31.527	6.164	13.544	1.00 26.52	A
MOTA	23	CB	HIS	A	5		30.939	6.339	14.950	1.00 25.34	A
MOTA	24	CG	HIS		5		30.240	7.647	15.156	1.00 28.69	A
ATOM	25		HIS		5		30.716	8.870	15.492	1.00 29.15	A
ATOM	26		HIS		5		28.881	7.801	14.979	1.00 28.23 1.00 29.92	A
MOTA	27		HIS		5 5		28.550 29.645	9.062 9.732	15.198 15.511	1.00 29.92	A A
ATOM ATOM	28 29	NE2	HIS		5		32.246	4.826	13.465	1.00 25.79	A
ATOM	30	0	HIS		5		31.630	3.785	13.227	1.00 25.68	A
ATOM	31	N	VAL		6		33.559	4.866	13.659	1.00 24.52	A
ATOM	32	CA	VAL		6		34.385	3.667	13.628	1.00 23.27	A
ATOM	33	CB	VAL		6		35.311	3.657	12.407	1.00 25.22	A
ATOM	34	CG1	VAL	A	6		36.187	2.414	12.440	1.00 24.31	A
ATOM	35	CG2	VAL	A	6		34.489	3.708	11.127	1.00 27.15	A
MOTA	36	С	VAL		6		35.256	3.633	14.876	1.00 22.15	A
ATOM	37	0	VAL		6		35.937	4.606	15.185	1.00 21.49 1.00 19.90	A A
MOTA	38	N	ALA		7 7		35.239 36.038	2.513 2.382	15.586 16.799	1.00 19.70	A
ATOM ATOM	39 40	CA CB	ALA ALA		7		35.132	2.394	18.034	1.00 14.59	A
ATOM	41	C	ALA		7		36.867	1.111	16.791	1.00 18.62	A
ATOM	42	ŏ	ALA		7		36.548	0.153	16.088	1.00 20.78	A
ATOM	43	N	SER		8		37.947	1.120	17.560	1.00 16.95	A
ATOM	44	CA	SER	A	8		38.807	-0.048	17.700	1.00 18.62	A
ATOM	45	CB	SER	A	8		40.211	0.215	17.153	1.00 17.69	A
MOTA	46	OG	SER		8		40.209	0.271	15,738	1.00 19.81	A
MOTA	47	C	SER		8		38.868	-0.310	19.199 19.943	1.00 18.76 1.00 19.35	A A
ATOM	48	0	SER		8		39.570 38.070	0.376 -1.268	19.645	1.00 19.38	Ā
ATOM ATOM	49 50	n Ca	TYR TYR		9 9		38.038	-1.608	21.048	1.00 19.44	A
ATOM	51	CB	TYR		9		36.628	-1.980	21.471	1.00 19.18	A
MOTA	52	CG	TYR		9		35.714	-0.785	21.375	1.00 18.65	A
ATOM	53		TYR		9		36.073	0.435	21.962	1.00 16.57	A
MOTA	54	CE1	TYR	A	9		35.237	1.537	21.897	1.00 17.39	A
MOTA	55	CD2	TYR	A	9		34.493	-0.865	20.716	1.00 17.15	A
MOTA	56	CE2	TYR		9		33.641	0.235	20.647	1.00 16.82	A
MOTA	57	CZ	TYR		9		34.020	1.431	21.243	1.00 18.07	A
MOTA	58	OH	TYR		9		33.169	2.509	21.210	1.00 19.77	A A
MOTA	59	C	TYR		9		38.993 38.652	-2.751	21.106 21.344	1.00 20.21 1.00 15.05	A
MOTA MOTA	60 61	o N	TYR GLY		9 10		40.225	-3.911 -2.357	20.831	1.00 15.05	A
ATOM	62	CA	GLY		10		41.311	-3.275	20.831	1.00 22.54	A
MOTA	63	C	GLY		10		42.276	-3.080	19.655		A
MOTA	64	Ö	GLY		10		42.248	-3.863	18.713	1.00 22.02	A
MOTA	65	N	VAL		11		43.083	-2.023	19.674	1.00 18.91	A
ATOM	66	CA	VAL		11		44.119	-1.949	18.651		A
MOTA	67	CB	VAL		11		44.554	-0.506	18.277		A
MOTA	68		VAL		11		45.845	-0.558	17.455		A
MOTA	69	CG2	VAL	A	11		43.481	0.165	17.432	1.00 15.25	A

ATOM	70	C	VAL A	11	45.228	-2.644	19.447	1.00 17.05	A
ATOM	71	0	VAL A	11	45.679	-2.145	20.481	1.00 19.34	A
MOTA	72	N	ASN A	12	45.616	-3.828	19.005	1.00 17.39	A
MOTA	73	CA	ASN A	12	46.643	-4.597	19.693	1.00 17.18	A
ATOM	74	CB ~~	ASN A	12	46.113	-5.994	20.052	1.00 15.04 1.00 15.96	A A
ATOM ATOM	75 76	CG OD1	ASN A	12 12	44.834 43.780	-5.947 -5.490	20.882 20.417	1.00 18.20	A
ATOM	77		ASN A	12	44.921	-6.420	22.114	1.00 10.46	A
ATOM	78	C	ASN A	12	47.863	-4.739	18.797	1.00 18.90	A
ATOM	79	0	ASN A	12	47.752	-5.162	17.641	1.00 18.80	A
ATOM	80	N	LEU A	13	49.026	-4.403	19.343	1.00 18.60	A
ATOM	81	CA	LEU A	13	50.264	-4.478	18.599	1.00 19.90	A
ATOM	82	CB	LEU A	13	50.695	-3.064	18.217	1.00 23.26	A
MOTA	83	CG	TEU Y		52.077	-2.881	17.594	1.00 24.86	A
ATOM	84		LEU A		52.085	-3.494	16.201	1.00 26.92	A
ATOM	85		LEU A		52.417	-1.402	17.534	1.00 24.75 1.00 20.37	A A
MOTA MOTA	86 87	0	TER Y		51.391 51.559	-5.165 -4.953	19.370 20.566	1.00 20.37	A
ATOM	88	N	TYR A		52.145	-6.004	18.673	1.00 21.04	A
ATOM	89	CA	TYR A		53.291	-6.691	19.255	1.00 24.07	A
ATOM	90	CB	TYR A		52.909	-8.050	19.844	1.00 27.05	A
MOTA	91	CG	TYR A	14	54.091	-8.729	20.489	1.00 29.27	A
ATOM	92	CD1	TYR A	14	54.569	-8.304	21.723	1.00 30.07	A
MOTA	93		TYR A		55.709	-8.867	22.285	1.00 31.38	A
ATOM	94		TYR A		54.783	-9.744	19.830	1.00 31.63	A
ATOM	95		TYR A			-10.314	20.383	1.00 30.29	A
ATOM	96		TYR A		56.381	-9.868	21.609	1.00 31.37 1.00 34.48	A A
ATOM	97	OH	TYR A		57.515 54.291	-10.413 -6.900	22.160 18.128	1.00 25.30	A
ATOM ATOM	98 99	С 0	TYR A		53.907	-7.206	16.994	1.00 25.51	A
MOTA	100	N	GLN A		55.571	-6.725	18.429	1.00 24.61	A
ATOM	101	CA	GLN A		56.603	-6.891	17.414	1.00 25.19	A
ATOM	102	CB	GLN A		56.932	-5.549	16.754	1.00 23.54	A
ATOM	103	CG	GLN A	. 15	57.278	-4.443	17.738	1.00 23.98	A
MOTA	104	CD	GLN A	. 15	57.567	-3.116	17.056	1.00 26.32	A
ATOM	105	OE1	GLN A		57.575	-2.062	17.702	1.00 28.26	A
ATOM	106	NB2			57.810	-3.159	15.749	1.00 24.64	A
ATOM	107	C	GLN A		57.848	-7.487	18.036	1.00 26.16	A
ATOM	108	0	GLN A		58.134	-7.263	19.211 17.236	1.00 24.31 1.00 28.72	A A
ATOM	109	N	SER A		58.583 59.801	-8.252 -8.912	17.698	1.00 30.37	A
MOTA MOTA	110 111	CA CB	SER A		60.341	-9.830	16.603	1.00 28.35	A
ATOM	112	og	SER A		60.569	-9.100	15.407	1.00 31.43	A
ATOM	113	c	SER A		60.883	-7.918	18.111	1.00 32.37	A
MOTA	114	0	SER A	16	61.538	-8.104	19.134	1.00 33.91	A
MOTA	115	N	TYR A	17	61.073	-6.863	17.325	1.00 32.49	A
MOTA	116	CA	TYR A		62.096	-5.890	17.664	1.00 34.27	A
MOTA	117	СВ	TYR A		62.172	-4.788	16.620	1.00 35.41	A
ATOM	118	CG	TYR A		63.371	-3.911	16.837	1.00 37.77 1.00 39.38	A A
ATOM	119		TYR A		64.646 65.769	-4.347 -3.569	16.470 16.715	1.00 40.15	Ā
MOTA MOTA	120 121		TYR		63.247	-2.671	17.456	1.00 36.31	A
ATOM	122	CE2	_		64.360	-1.886	17.707	1.00 39.40	A
ATOM	123	CZ	TYR A		65.621	-2.338	17.335	1.00 41.42	A
ATOM	124	OH	TYR A		66.732	-1.562	17.580	1.00 43.02	A
ATOM	125	C	TYR A	17	61.821	-5.270	19.027	1.00 34.43	A
ATOM	126	0	TYR A		60.765	-4.682	19.248	1.00 35.58	A
MOTA	127	N	GLY A		62.783	-5.390	19.935	1.00 34.98	A
MOTA	128	CA	GLY 1		62.609	-4.854	21.270	1.00 35.78 1.00 36.87	A A
ATOM	129	C	GLY 1		62.730 63.761		22.292 22.952	1.00 38.48	A
ATOM	130 131	O N	GLY I		61.692		22.459	1.00 37.06	A
MOTA MOTA	132	CD	PRO I		61.745		23.368	1.00 35.58	A
MOTA	133	CA	PRO 2		60.409		21.747	1.00 34.79	A
ATOM	134	СВ	PRO 2		59.853		21.981	1.00 35.91	A
MOTA	135	CG	PRO 2		60.300		23.394	1.00 36.88	A
MOTA	136	C	PRO 2	A 19	59.531		22.379	1.00 33.10	A
MOTA	137	0	PRO 2		59.844		23.456	1.00 33.71	A
MOTA	138	N	SER		58.435		21.722	1.00 31.83	A
MOTA	139	CA	SER		57.548		22.290	1.00 30.25 1.00 29.00	A A
MOTA	140	CB OG	SER .		58.060 58.072		21.965 20.567	1.00 23.00	A
ATOM ATOM	141 142	C	SER .		56.108			1.00 27.93	A
MOTA	143	Ö	SER .		55.829		20.805	1.00 28.23	A
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ATOM	144	N	GLY	A	21	55.191	-3.911	22.576	1.00 25.87	A
ATOM	145	CA	GLY		21	53.797		.22,222	1.00 23.78	A
ATOM	146	c	GLY		21	53.076	-2.732	22.598	1.00 23.94	A
ATOM	147	0	GLY		21	53.638	-1.840	23.247	1.00 24.81	A
MOTA	148	N	GLN	A	22	51.821	-2.641	22.187	1.00 20.60	A
MOTA	149	CA	GLN	A	22	51.033	-1.470	22.495	1.00 19.67	A
MOTA	150	CB	GLN		22	51.239	-0.400	21.415	1.00 19.28	A
MOTA	151	CG	GLN		22	50.584	0.943	21.736	1.00 18.12	A
MOTA	152	CD	GLN		22	50.732	1.971	20.613	1.00 18.84	A
MOTA	153		GLN		22	51.694	2.749	20.576	1.00 19.77	A A
ATOM	154		GLN		22	49.777 49.573	1.968 -1.873	19.688 22.566	1.00 16.83 1.00 18.66	A
ATOM	155	C	GLN		22 22	49.128	-2.747	21.826	1.00 18.45	A
ATOM	156 157	N N	TYR		23	48.842	-1.257	23.484	1.00 17.25	A
MOTA MOTA	158	CA	TYR		23	47.423	-1.529	23.615	1.00 16.53	A
ATOM	159	CB	TYR		23	47.127	-2.497	24.752	1.00 14.51	A
MOTA	160	CG	TYR		23	45.674	-2.904	24.760	1.00 12.67	A
MOTA	161		TYR	A	23	45.251	-4.070	24.121	1.00 13.38	A
MOTA	162	CE1	TYR	A	23	43.904	-4.415	24.070	1.00 13.23	A
MOTA	163	CD2	TYR	A	23	44.713	-2.093	25.346	1.00 11.07	A
MOTA	164		TYR		23	43.365	-2.425	25.299	1.00 12.99	A A
MOTA	165	CZ	TYR		23	42.964	-3.583	24.664 24.611	1.00 13.72 1.00 17.15	A
MOTA	166	OH	TYR		23	41.624 46.694	-3.907 -0.220	23.860	1.00 16.88	A
MOTA	167	C	TYR		23 23	46.975	0.491	24.824	1.00 16.57	A
ATOM ATOM	168 169	Ŋ	THR		24	45.757	0.085	22.969	1.00 16.16	A
MOTA	170	CA	THR		24	44.975	1.311	23.038	1.00 16.43	A
MOTA	171	СВ	THR		24	45.594	2.405	22.136	1.00 18.41	A
ATOM	172		THR		24	45.581	1.954	20.771	1.00 17.20	A
ATOM	173	CG2	THE	A	24	47.029	2.692	22.537	1.00 18.64	A
ATOM	174	C	THE	A	24	43.570	1.058	22.499	1.00 15.15	A
MOTA	175	0	THE		24	43.314	0.037	21.879	1.00 15.70 1.00 15.66	A A
MOTA	176	N	HIS		25	42.667	1.993 1.924	22.754 22.210	1.00 15.79	A
ATOM	177	CA	HIS		25 25	41.320 40.243	1.834	23.297	1.00 13.55	A
MOTA MOTA	178 179	CB	HIS		25	39.956	0.430	23.734	1.00 15.91	A
ATOM	180		HIS		25	40.688	-0.704	23.624	1.00 13.86	A
ATOM	181		HIS		25	38.790	0.071	24.374	1.00 15.91	A
ATOM	182	CE1	HIS	A	25	38.815	-1.222	24.639	1.00 14.38	A
ATOM	183	NE2	HIS	A	25	39.956	-1.715	24.193	1.00 16.99	A
MOTA	184	C		S A	25	41.176	3.212	21.437	1.00 14.18	A A
ATOM	185	0		3 A	25	41.677	4.241 3.150	21.865 20.292	1.00 13.52 1.00 14.81	A
ATOM	186	N		J A J A	26 26	40.510 40.333	4.329	19.462	1.00 16.96	A
MOTA MOTA	187 188	CA CB		JA	26	41,132	4.188	18.164	1.00 16.34	A
ATOM	189	CG	_	JA	26	42.644	4.158	18.311	1.00 18.80	A
MOTA	190	CD		JA	26	43.345	4.036	16.958	1.00 22.68	A
ATOM	191	OE	LGL	J A	26	42.744	4.456	15.946	1.00 26.77	A
MOTA	192	OE:	GL	υA	26	44.490	3.539	16.901	1.00 20.46	A
MOTA	193	C		A U	26	38.875	4.543	19.101	1.00 17.22	A
MOTA	194	0		UA		38.104	3.597	18.996	1.00 18.66 1.00 18.91	A A
MOTA	195	N		E A	27	38.503 37.150	5.802 6.135	18.917 18.509	1.00 19.32	A
MOTA	196	CA		B A E A		36.290	6.546		1.00 20.19	A
MOTA MOTA	197 198	CB		ΒA		34.834	6.653		1.00 23.33	A
MOTA	199		1 PH			34.024	5.524			A
MOTA	200		2 PH			34.289	7.868	18.971		A
MOTA	201		1 PH			32.692	5.606	18.980		A
MOTA	202	CE	2 PH	E A	. 27	32.954	7.962			A
MOTA	203	CZ	PH	E A		32.155	6.828			A
MOTA	204	C		EA		37.260	7.291			A A
ATOM	205			EA		37.733	8.375			A
MOTA	206			PA		36.831				Ā
MOTA	207			P A		36.901 35.910				A
MOTA	208 209			PA		34.472				A
ATOM ATOM	210		1 AS			34.266				A
ATOM	211		2 AE			33.552			1.00 27.42	A
MOTA	212			P		38.297		15.043		A
ATOM	213		AS	SP A	28	38.467				A
MOTA	214	N		Y Z		39.292				A
MOTA	215			Y		40.658				A A
ATOM	216			Y		41.437				A
ATOM	217	7 0	GI	ZX 1	A 29	42.621	9.010	, 13.014		••

ATOM	218	N	ASP	A	30	40.797	8.922	17.098	1.00 16.92	A
MOTA	219	CA	ASP		30	41.511	9.438	18.254	1.00 16.83	A
MOTA	220	СВ	ASP		30	40.816 40.988	10.678 11.864	18.796 17.888	1.00 18.99 1.00 21.09	A A
ATOM ATOM	221 222	CG	ASP ASP		30 30	42.145	12.177	17.538	1.00 22.94	A
ATOM	223		ASP		30	39.971	12.478	17.525	1.00 21.68	A
ATOM	224	C	ASP		30	41.656	8.392	19.345	1.00 17.25	A
ATOM	225	0	ASP	A	30	40.777	7.553	19.543	1.00 15.40	A
MOTA	226	N	ĠΓΩ		31	42.784	8.453	20.041	1.00 16.77	A
MOTA	227	CA	Gra		31	43.111	7.514	21.107	1.00 18.43	A
MOTA	228	CB	GLU		31	44.620 45.147	7.607 6.853	21.392 22.608	1.00 20.90 1.00 24.68	A A
ATOM ATOM	229 230	CG CD	Gra Gra		31 31	46.678	6.924	22.702	1.00 27.25	A
ATOM	231		GLU		31	47.258	7.931	22.239	1.00 26.93	A
MOTA	232		GLU		31	47.302	5.985	23.242	1.00 27.21	A
ATOM	233	C	GLU	A	31	42.296	7.777	22.375	1.00 17.51	A
MOTA	234	0	GΓΩ		31	42.361	8.863	22.952	1.00 17.13	A
MOTA	235	N	GLN		32	41.525 40.726	6.784 6.942	22.807 24.020	1.00 15.52 1.00 16.47	A A
MOTA	236 237	CA CB	GLN GLN		32 32	39.542	5.980	24.009	1.00 15.91	A
ATOM ATOM	238	CG	GLN		32	38.439	6.399	23.065	1.00 15.97	A
ATOM	239	CD	GLN		32	37.292	5.419	23.071	1.00 20.20	A
ATOM	240	OE1	GLN	A	32	37.478	4.228	22.808	1.00 18.09	A
MOTA	241	NE2			32	36.091	5.912	23.374	1.00 20.57	A
ATOM	242	C	GLN		32	41.584	6.701	25.255 26.272	1.00 16.61 1.00 15.51	A A
ATOM	243	0	GLN		32	41.448 42.470	7.387 5.720	25.151	1.00 15.59	A
MOTA MOTA	244 245	N CA	PHE		33 33	43.370	5.389	26.239	1.00 16.34	A
MOTA	246	CB	PHE		33	42.583	4.854	27.443	1.00 17.21	A
ATOM	247	CG	PHE	A	33	41.951	3.502	27,222	1.00 16.68	A
ATOM	248		PHE		33	42.686	2.333	27.406	1.00 15.57	A
MOTA	249		PHE		33	40.598	3.397	26.903	1.00 18.54	A A
ATOM	250	-	PHE		33 33	42.083 39.983	1.076 2.147	27.288 26.782	1.00 16.34 1.00 17.35	A
ATOM ATOM	251 252	CEZ	PHE PHE		33	40.729	0.983	26.978	1.00 16.56	A
ATOM	253	C	PHE		33	44.363	4.343	25.776	1.00 16.66	A
ATOM	254	o	PHE		33	44.209	3.746	24.712	1.00 16.85	A
ATOM	255	N	TYF	R S	34	45.398	4.139	26.572	1.00 16.03	A
ATOM	256	CA	TYF		34	46.377	3.125	26.264	1.00 16.93	A
MOTA	257	СВ		R A	34	47.636	3.730	25.621 26.523	1.00 16.33 1.00 17.31	A A
ATOM	258	CG	TYI IYT J	A S	34 34	48.528 49.519	4.541 3.930	27.291	1.00 17.48	A
MOTA MOTA	259 260		L TY		34	50.367	4.683	28.097	1.00 19.16	A
ATOM	261		TY		34	48.404	5.928	26.586	1.00 17.68	A
MOTA	262		TYI		34	49.244	6.690	27.388	1.00 19.73	A
MOTA	263	CZ		R A	34	50.224	6.060	28.141	1.00 20.10	A
MOTA	264	OH		R A	34	51.044	6.815	28.941	1.00 23.02 1.00 17.88	A A
MOTA	265	C		R A R A	34 34	46.692 46.429	2.473 3.042	27.588 28.646	1.00 21.13	A
MOTA MOTA	266 267	N O		LA	35	47.213	1.261	27.535	1.00 17.31	A
MOTA	268	CA		LА	35	47.571	0.570	28.749	1.00 18.89	A
MOTA	269	CB	VA	L A	35	46.950	-0.848	28.804	1.00 19.12	A
MOTA	270		1 VA			47.589	-1.660	29.912	1.00 17.56	A
MOTA	271		2 VA			45.454				A A
MOTA	272			L A L A		49.084 49.701				A
MOTA	273 274			и Р A		49.676				A
ATOM ATOM	275			PA		51.121				A
ATOM	276			PA		51.542	1.872	31.172		A
MOTA	277	CG		PA		53.033		_		A
MOTA	278		1 AS			53.796				A A
MOTA	279		2 AS	PA		53.441 51.393				A
MOTA MOTA	280 281			PA		51.016				A
ATOM	282			T P		52.024		_		A
MOTA	283			U Z		52.305	-2.600	29.588	1.00 29.51	A
MOTA	284		LE	T DE		52.754				A
MOTA	285			T A		51.704				A
MOTA	286		1 LE			52.269				A A
MOTA	287		2 LE	3U 2 3U 2		50.455 53.348				A
ATOM ATOM	288 289			3U 1		53.222				A
ATOM	290			ZY Z		54.362				A
MOTA	291			LY I		55.403		31.73	7 1.00 35.44	A
								27		
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MOTA	292	С	GLY	A	38	54.956	-1.863	33.162	1.00 37.63	A
MOTA	293	0	GLY		38	55.369	-2.549	34.098	1.00 38.42	A
MOTA	294	N	ARG		39	54.101	-0.861	33.334	1.00 38.93	A A
MOTA	295	CA	ARG		39	53.625 53.645	-0.499 1.029	34.660 34.803	1.00 40.81 1.00 42.41	A
MOTA	296 297	CB CG	ARG ARG		39 39	54.968	1.627	34.339	1.00 44.76	A
MOTA MOTA	298	CD	ARG		39	55.113	3.118	34.619	1.00 47.83	A
ATOM	299	NE	ARG		39	56.318	3.644	33.976	1.00 50.52	A
ATOM	300	CZ	ARG	A	39	56.902	4.799	34.281	1.00 53.40	A
MOTA	301	NHl			39	56.399	5.575	35.235	1.00 54.01	A
MOTA	302	NH2	ARG		39	57.998	5.179	33.633 34.936	1.00 54.18 1.00 41.12	A A
ATOM	303	C	ARG		39 39	52.229 51.664	-1.057 -0.847	36.014	1.00 39.71	A
ATOM	304 305	N O	ARG		40	51.687	-1.779	33.955	1.00 40.65	A
ATOM ATOM	305	CA	LYS		40	50.365	-2.380	34.070	1.00 39.55	A
ATOM	307	СВ	LYS		40	50.415	-3.554	35.053	1.00 42.42	A
ATOM	308	CG	LYS	A	40	49.196	-4.467	34.996	1.00 46.46	A
ATOM	309	CD	LYS		40	49.266	-5.563	36.054	1.00 50.42	A
MOTA	310	CE	LYS		40	48.077	-6.513	35.947	1.00 51.25 1.00 52.15	A A
ATOM	311	NZ	LYS		40	46.781 49.338	-5.779 -1.348	35.970 34.540	1.00 37.45	A
ATOM	312 313	С 0	LYS		40 40	48.647	-1.560	35.533	1.00 35.78	A
MOTA MOTA	314	N	GLU		41	49.245	-0.237	33.812	1.00 35.81	A
ATOM	315	CA	GLU		41	48.317	0.847	34.142	1.00 33.83	A
ATOM	316	CB	GLU	A	41	49.077	2.079	34.655	1.00 36.46	A
MOTA	317	ÇG	GLU		41	49.660	1.997	36.049	1.00 41.33	A A
MOTA	318	CD	GLU		41	50.500	3.224	36.374 36.022	1.00 44.23 1.00 46.67	A
MOTA	319		GLU		41 41	50.067 51.585	4.343 3.076	36.981	1.00 45.55	A
ATOM ATOM	320 321	OE2	GLU		41	47.492	1.301	32.937	1.00 30.89	A
ATOM	322	Ö	GLU		41	47.995	1.373	31.816	1.00 27.89	A
ATOM	323	N	THE		42	46.227	1.623	33.182	1.00 28.11	A
ATOM	324	CA	THE	A	42	45.354	2.127	32.135	1.00 26.58	A
ATOM	325	CB	THE		42	43.882	1.773	32.406	1.00 27.67	A A
MOTA	326		THE		42	43.716	0.349 2.419	32.394 31.357	1.00 25.55 1.00 25.33	A
MOTA	327		THE		42 42	42.979 45.506	3.642	32.212	1.00 26.90	A
MOTA MOTA	328 329	C	THE		42	45.305	4.232	33.269	1.00 25.79	A
MOTA	330	N	VAI		43	45.881	4.273	31.108	1.00 25.87	A
ATOM	331	CA		A	43	46.045	5.720	31.106	1.00 24.36	A
MOTA	332	СВ		A	43	47.474	6.119	30.670	1.00 24.45	A
MOTA	333	CG1		L A	43	47.698	7.606	30.906 31.433	1.00 24.38 1.00 22.82	A A
MOTA	334		VAI		43	48.504 45.039	5.289 6.331	30.141	1.00 24.94	A
ATOM	335 336	С 0		L A L A	43 43	45.143	6.133	28.930	1.00 24.72	A
ATOM ATOM	337	N		PA	44	44.063	7.065	30.672	1.00 24.50	A
ATOM	338	CA		РΑ	44	43.050	7.681	29.824	1.00 25.64	A
ATOM	339	CB	TR	PΑ	44	41.804	8.033	30.642	1.00 25.03	A
MOTA	340	ÇG		PA	44	41.224	6.859	31.370	1.00 25.96 1.00 25.77	A A
MOTA	341		2 TR		44	40.281	5.906 4.946	30.858 31.870	1.00 26.64	A
ATOM	342		2 TR 3 TR		44 44	40.067	5.766	29.641	1.00 24.94	A
MOTA MOTA	343 344		1 TR		44	41.529		32.634	1.00 26.43	A
ATOM	345		1 TR			40.840	5.305	32.942	1.00 26.28	A
MOTA	346		2 TR			39.197			1.00 25.00	A
MOTA	347		3 TR			38.734			1.00 22.40 1.00 24.18	A A
ATOM	348		2 TR	PA PA		38.542			1.00 26.30	A
MOTA	349 350			P A		43.578 44.321				A
MOTA MOTA	351			SA		43.193				A
MOTA	352			SA		43.635		27.062		A
MOTA	353	СВ		SA		44.069				A A
MOTA	354			SA		45.547	_			A A
MOTA	355			SA		42.574				A
MOTA	356			rs a Su a		42.836 41.375				A
MOTA MOTA	357 358			SU A		40.26				A
ATOM	359			SU P		39.13	7 11.493	26.506		A
MOTA	360	CG		SU P		38.81				A A
MOTA	361		1 L			37.49				A A
MOTA	362)2 Li	3U <i>1</i> 3U <i>1</i>		38.710 39.73				A
ATOM ATOM	363 364			EU 2		39.19				A
ATOM	369			RO 2		39.89				A

ATOM	366	CD	PRO	20.	47	40.488	14.442	28.986	1.00 32.23	A
ATOM	367	CA	PRO		47	39.437	13.392	30.901	1.00 32.18	A
	368	CB	PRO		47	39.487	14.908	31.063	1.00 32.11	A
ATOM								30.236	1.00 31.60	A
MOTA	369	CG	PRO		47	40.690	15.270			A
MOTA	370	C	PRO		47	38.066	12.800	31.245	1.00 30.96	A
ATOM	371	0	PRO		47	37.927	12.103	32.243	1.00 30.17	
MOTA	372	N	VAL		48	37.064	13.068	30.418	1.00 30.75	A
MOTA	373	CA	VAL		48	35.715	12.563	30.663	1.00 32.56	A
ATOM	374	CB	VAL		48	34.748	13.040	29.560	1.00 34.04	A
MOTA	375		VAL		48	33.320	12.683	29.932	1.00 34.16	A
MOTA	376	CG2	VAL	A	48	34.881	14.556	29.368	1.00 38.02	A
ATOM	377	С	VAL	A	48	35.633	11.033	30.765	1.00 33.13	A
MOTA	378	0	VAL	A	48	34.698	10.485	31.355	1.00 33.55	A
ATOM	379	N	LEU	A	49	36.615	10.350	30.192	1.00 33.30	A
MOTA	380	CA	LEU	A	49	36.661	8.892	30.208	1.00 32.44	A
ATOM	381	CB	LEU	A	49	37.498	8.391	29.023	1.00 30.62	A
ATOM	382	CG	LEU		49	36.792	8.027	27.702	1.00 31.64	A
	383		LEU		49	35.578	8.888	27.464	1.00 29.12	A
MOTA	384		LEU		49	37.783	8.157	26.551	1.00 31.05	A
ATOM	385	c	LEU		49	37.226	8.343	31.519	1.00 33.77	A
ATOM	386	ō	LEU		49	37.138	7.142	31.787	1.00 34.14	A
			ARG		50	37.794	9.221	32.339	1.00 34.56	A
ATOM	387	N			50	38.367	8.810	33.618	1.00 35.58	A
ATOM	388	CA	ARG					34.345	1.00 37.99	A
ATOM	389	СВ	ARG		50	38.987	10.009			A
MOTA	390	CG	ARG		50	40.137	10.720	33.636	1.00 40.65	
MOTA	391	œ	ARG		50	40.657	11.846	34.529	1.00 43.05	A
MOTA	392	NE	ARG		50	41.603	12.748	33.872	1.00 44.85	A
MOTA	393	CZ	ARG		50	42.815	12.403	33.444	1.00 46.08	A
MOTA	394	NH1	ARG	A	50	43.254	11.159	33.592	1.00 46.76	A
MOTA	395	NH2	ARG	A	50	43.599	13.314	32.880	1.00 46.08	A
ATOM	396	C	ARG	A	50	37.334	8.168	34.547	1.00 35.55	A
MOTA	397	0	ARG	A	50	37.693	7.475	35.495	1.00 35.21	A
ATOM	398	N	GLN	A	51	36.054	8.412	34.284	1.00 36.77	A
ATOM	399	CA	GLN	A	51	34.987	7.859	35.116	1.00 37.34	A
ATOM	400	СВ	GLN		51	33.658	8.558	34.821	1.00 39.02	A
ATOM	401	CG	GLN		51	33.123	8.306	33.418	1.00 41.24	A
MOTA	402	CD	GLN.		51	31.765	8.947	33.189	1.00 43.49	A
MOTA	403		GLN		51	30.781	8.597	33.843	1.00 43.80	A
ATOM	404	NE2			51	31.706	9.895	32.260	1.00 44.01	A
			GLN		51	34.821	6.362	34.896	1.00 36.85	A
ATOM	405	C					5.665	35.734	1.00 37.06	A
ATOM	406	0	GLN		51	34.250		33.764	1.00 37.00	A
MOTA	407	N	PHE		52	35.316	5.871			A
MOTA	408	CA	PHE		52	35.218	4.454	33.446	1.00 32.82	
MOTA	409	CB	PHE		52	35.143	4.258	31.931	1.00 31.28	A
MOTA	410	CG	PHE		52	33.902	4.838	31.301	1.00 29.86	A
MOTA	411		PHE		52	32.640	4.549	31.821	1.00 27.82	A
MOTA	412		PHE		52	33.992	5.652	30.177	1.00 27.71	A
MOTA	413		PHE		52	31.490	5.060	31.234	1.00 25.58	A
MOTA	414	CE2	PHE	A	52	32.847	6.171	29.580	1.00 28.10	A
MOTA	415	CZ	PHE	A	52	31.592	5.873	30.111	1.00 28.21	A
ATOM	416	C	PHE	A	52	36.405	3.675	34.004	1.00 32.57	A
ATOM	417	0	PHE	A	52	37.370	4.256	34.494	1.00 32.22	A
ATOM	418	N	ARG		53	36.327	2.353	33.927	1.00 32.80	A
ATOM	419	CA	ARG		53	37.397	1.498	34.419	1.00 32.77	A
MOTA	420	CB	ARG		53	37.005	0.862	35.760	1.00 36.56	A
ATOM	421	CG	ARG		53	36.741	1.867	36.881	1.00 42.83	A
ATOM	422	CD	ARG		53	36.523	1.168	38.214	1.00 49.04	A
	423	NE	ARG		53	36.308	2.111	39.312	1.00 53.82	A
MOTA			ARG			36.195	1.758	40.589	1.00 54.70	A
MOTA	424	CZ			53		0.478	40.937	1.00 55.50	A
MOTA	425		ARG		53	36.277	2.683	41.520	1.00 55.64	A
MOTA	426		ARG		53	36.004				Ā
MOTA	427	C	ARG		53	37.706	0.404	33.405	1.00 29.88	
MOTA	428	0	ARG		53	36.806	-0.117	32.743	1.00 28.71	A
MOTA	429	N	PHE		54	38.986		33.293	1.00 26.44	A
MOTA	430	CA	PHE		54	39.440			1.00 22.47	A
MOTA	431	CB	PHE		54	39.905			1.00 21.88	A
MOTA	432	CG	PHE		54	40.181			1.00 20.69	A
ATOM	433	CD:	L PHE	A	54	39.150			1.00 19.52	A
ATOM	434	CD:	2 PHE	A	54	41.471			1.00 18.68	A
ATOM	435	CE:	L PHE	A	54	39.399	-2.734	28.170	1.00 22.81	A
MOTA	436	CE	2 PHE	A S	54	41.733		28.746		A
MOTA	437	CZ	PHE		54	40.697	-3.190	27.954	1.00 20.86	A
MOTA	438	C	PHE		54	40.597				A
ATOM	439		PHI		54	41.631			1.00 23.53	A

MOTA	440	N	ASP	A	55	40.408	-3.011	33.198	1.00 22.82	A
ATOM	441	CA	ASP		55	41.411	-3.874	33.805	1.00 24.70	A
	442	CB	ASP		55	40.785	-5.246	34.083	1.00 23.26	A
ATOM		CG	ASP		55	41.729	-6.190	34.789	1.00 26.24	A
ATOM	443		ASP		55	42.924	-5.853	34.933	1.00 28.75	A
ATOM	444		ASP		55	41.274	-7.279	35.192	1.00 26.38	A
ATOM	445		ASP		55	42.613	-4.011	32.861	1.00 24.24	A
ATOM	446	C			55	42.510	-4.629	31.802	1.00 23.91	A
ATOM	447	0	ASP			43.770	-3.437	33.238	1.00 23.69	A
MOTA	448	И	PRO		56		-2.761	34.509	1.00 23.79	A
ATOM	449	Œ	PRO		56	44.084	-3.522	32.387	1,00 23.45	A
ATOM	450	CA	PRO		56	44.961 46.002	-2.707	33.162	1.00 23.35	A
ATOM	451	CB	PRO		56			34.580	1.00 23.31	A
MOTA	452	CG	PRO		56	45.592	-2.897 -4.952		1.00 23.66	A
ATOM	453	C	PRO		56	45.413		32.114 31,125	1.00 23.15	A
MOTA	454	0	PRO		56	46.099	-5.220	32.991	1.00 21.84	Ā
MOTA	455	N	GLN		57	45.025	-5.871	32.818	1.00 22.47	A
ATOM	456	CA	GLN		57	45.397	-7.261	33.965	1.00 23.11	A
ATOM	457	CB	GITN		57	44.834	-8.108		1.00 20.82	A
ATOM	458	CG	GLN		57	45.226	-9.568	33.873	1.00 20.82	A
MOTA	459	CD	GLN		57	46.722	-9.745	33.733	1.00 21.88	A
ATOM	460		GLN		57 	47.497	-9.227	34.539	1.00 23.15	A
ATOM	461		GLN		57	47.138		32.707 31.482	1.00 22.21	A
ATOM	462	C	GLN		57	44.882	-7.792		1.00 23.00	A
ATOM	463	0	GLN		57	45.452	-8.723	30.913	1.00 23.00	A
MOTA	464	N	PHE		58	43.801	-7.203	30.980	1.00 21.07	A
ATOM	465	CA	PHE		58	43.254	-7.640	29.704	1.00 20.45	A
MOTA	466	CB	PHE		58	42.004	-6.857	29.338	1.00 20.43	Ā
MOTA	467	CG	PHE		58	41.411	-7.287	28.031	1.00 18.42	A
MOTA	468		PHE		58	40.472	-8.312	27.988		A
MOTA	469		PHE		58	41.864	-6.736	26.835	1.00 18.79	Ā
MOTA	470		PHE		58	39.992	-8.792	26.765	1.00 21.25	A
MOTA	471		PHE		58	41.393	-7.207	25.610	1.00 20.28	A
MOTA	472	CZ	PHE		58	40.457	-8.238	25.578	1.00 21.18	A
MOTA	473	C	PHE		58	44.278	-7.401	28.612	1.00 21.79	
MOTA	474	0	PHE		58	44.529	-8.260	27.763	1.00 21.84	A
MOTA	475	N	ALA		59	44.849	-6.202	28.637	1.00 21.80	A
ATOM	476	CA	ALA		59	45.840	-5.801	27.657	1.00 21.67	A
MOTA	477	CB	ALA		59	46.254	-4.346	27.892	1.00 21.11	A
MOTA	478	C	ALA		59	47.053	-6.711	27.732	1.00 22.06	A
ATOM	479	0	ALA		59	47.518	-7.213	26.706	1.00 22.53	A
MOTA	480	N	LEU		60	47.561	-6.925	28.945	1.00 19.83	A
ATOM	481	CA	LEU		60	48.729	-7.777	29.116	1.00 20.88	A
MOTA	482	CB	LEU		60	49.163	-7.815	30.585	1.00 20.57	A
MOTA	483	CG	LEU		60	50.060	-6.657	31.053	1.00 24.17	A
ATOM	484		LEC.		60	49.239	-5.392	31.205	1.00 24.16	A
ATOM	485	CD	LEU		60	50.717	-7.012	32.382	1.00 24.31	A
MOTA	486	C	LEU		60	48.496	-9.193	28.598	1.00 20.44	A
MOTA	487	0	LEC		60	49.367	-9.770	27.955	1.00 21.97	A
MOTA	488	N	THE		61	47.319	-9.749	28.871	1.00 20.69	A
ATOM	489	ÇA	THE		61		-11.101	28.418	1.00 19.49	A
MOTA	490	CB	THE	A S	61		-11.629	29.084	1.00 18.59	A
MOTA	491	OG:			61		-11.830	30.489	1.00 21.12	A
MOTA	492		2 THE		61		-12.942	28.453	1.00 17.61	A
MOTA	493	C		R S	61		-11.140	26.903	1.00 19.22	A
MOTA	494	0		R S	61		-12.059	26.242	1.00 21.19	A
MOTA	495	N		A D	62		-10.142	26.351	1.00 18.05	A
ATOM	496	CA		A V			-10.092	24.910	1.00 19.26	A
MOTA	497			A V	62	45.020	-8.910	24.552	1.00 20.51	A
MOTA	498	CG		A R		43.835	-9.324	23.680	1.00 22.06	A
MOTA	499		1 AS				-10.482	23.693	1.00 21.71	A
MOTA	500		2 ASI			43.294	-8.371	22.930		A
MOTA	501	C	AS)	A n	62	47.270	-9.975			A
ATOM	502			A N			-10.681			A
MOTA	503			ВА		48.146	-9.108			A
ATOM	504			B A		49.448	-8.921			A
ATOM	505			e a		50.229	-7.757			A
MOTA	506		2 IL			51.601	-7.590			A
MOTA	507		1 IL			49.425	-6.457			A
MOTA	508		1 IL			49.037				A
MOTA	509			E A			-10.212			A
MOTA	510			E A			-10.538			A
MOTA	511			A A			-10.949			A
MOTA	512			A A			-12.222			A
ATOM	513	CE	AL	A A	64	50.373	-12.816	26.785	1.00 22.29	A

ATOM	514	C	ALA A	64	50.252 -		24.301	1.00 23.03	A
MOTA	515	0	ALA A	64	51.032 -		23.766	1.00 25.08	A
ATOM	516	N	VAL A	65	48.976 -		23.948	1.00 23.28	A A
MOTA	517	CA	VAL A	65 65	48.437 - 46.887 -		22.888 22.859	1.00 22.97 1.00 24.28	A
ATOM ATOM	518 519	CB	VAL A	65	46.338 -		21.729	1.00 22.40	A
ATOM	520		VAL A	65	46.325 -		24.209	1,00 19.61	A
ATOM	521	c	VAL A	65	49.013 -		21.538	1.00 23.88	A
ATOM	522	Õ	VAL A	65	49.313 -		20.692	1.00 22.01	A
ATOM	523	N	LEU A	66	49.179 -	12.164	21.332	1.00 24.00	A
ATOM	524	CA	LEU A	66	49.747 -	11.692	20.064	1.00 24.66	A
MOTA	525	CB	LEU A	66	49.872 -		20.011	1.00 22.13	A
MOTA	526	CG	LEU A	66		-9.228	20.117	1.00 23.81	A
MOTA	527		LEU A	66		-8.001	19.277	1.00 20.24	A
ATOM	528	-	LEU A	66	47.407 51.143 -	-9.866	19.627 19.906	1.00 20.49	A A
ATOM	529	0	LEU A	66 66	51.548 -		18.813	1.00 22.08	A
MOTA MOTA	530 531	N	LYS A	67	51.879 -		21.011	1.00 26.17	A
ATOM	532	CA	LYS A	67	53.237 -		21.019	1.00 28.99	A
MOTA	533	СВ	LYS A	67	53.839 -		22.421	1.00 29.27	A
ATOM	534	CG	LYS A	67	55.278 -	13.174	22.548	1.00 30.64	A
MOTA	535	CD	LYS A	67	55.779 -	13.001	23.976	1.00 32.41	A
ATOM .	536	CE	LYS A		57.159 -		24.157	1.00 35.25	A
MOTA	537	NZ	LYS A		58.144 -		23.199	1.00 38.78	A
ATOM	538	C	LYS A		53.200 -		20.598	1.00 29.87 1.00 30.35	A A
ATOM	539	0	LYS A		53.952 -		19.716 21.230	1.00 30.35	A
ATOM	540	N	HIS A		52.313 - 52.163 -		20.922	1.00 31.95	A
ATOM ATOM	541 542	CA CB	HIS A		51.051 -		21.775	1.00 34.42	A
MOTA	543	CG	HIS A		50.827 -		21.520	1.00 38.63	A
ATOM	544		HIS A		. 49.859 -		20.826	1.00 40.18	· A
ATOM	545	ND1	HIS A	68	51.676 -	-19.536	21.992	1.00 41.00	A
ATOM	546	CEl	HIS A	. 68	51.241 -		21.601	1.00 39.93	A
MOTA	547		HIS A		50.141 -		20.891	1.00 39.69	A
MOTA	548	C	HIS A			-16.660		1.00 31.53	A A
ATOM	549	0	HIS A		52.463 -		18.746	1.00 32.07 1.00 29.53	A
ATOM	550	N	ASN A		50.826 - 50.427 -		18.977 17.583	1.00 29.99	A
MOTA MOTA	551 552	CA CB	ASN A		49.180 -		17.332	1.00 30.27	A
ATOM	553	CG	ASN A		47.918 -		17.885	1.00 31.83	A
ATOM	554		ASN A		47.986 -		18.703	1.00 32.19	A
ATOM	555		ASN A		46.759 -	-15.328	17.447	1.00 31.41	A
MOTA	556	C	ASN A	69	51.552 -		16.638	1.00 30.37	A
MOTA	557	0	asn a		51.722 ·		15.571	1.00 29.41	A
ATOM	558	N	LEU A		52.324		17.026	1.00 29.86 1.00 31.35	A A
ATOM	559	CA	LEU A		53.413 · 54.039 ·		16.175 16.751	1.00 28.55	A
MOTA	560	CB CG	LEU A		55.190		15.950	1.00 28.77	A
ATOM ATOM	561 562		LEU A		54.745		14.519	1.00 28.48	A
MOTA	563		LEU A		55.651		16.627	1.00 27.89	A
ATOM	564	C	LEU A		54.479	-15.214	16.009	1.00 31.92	A
ATOM	565	0	LBU A	70	54.994	-15.422	14.914	1.00 31.72	A
MOTA	566	N	asn A		54.798		17.097	1.00 34.09	A
MOTA	567	CA	asn A		55.801		17.060	1.00 38.27	A
MOTA	568	CB	ASN A		55.884		18.427	1.00 39.70 1.00 44.05	A A
MOTA	569	CG	ASN A		56.490 56.290	-16.748	19.490 20.693	1.00 44.98	A
ATOM	570 571		lasni Lasni		57.247		19.049	1.00 44.44	A
MOTA MOTA	572	C KD	ASN A		55.484		15.983	1.00 38.32	A
ATOM	573	ō	ASN I			-18.417	15.224	1.00 37.91	. A
ATOM	574	N	SER A		54.221	-18.407	15.919	1.00 39.49	A
ATOM	575	CA	SER A	A 72		-19.390	14.944	1.00 40.10	A
ATOM	576	CB	SER A	A 72		-19.816	15.256	1.00 41.05	A
ATOM	577	OG	SER 2			-20.763	14.311	1.00 42.44	A
ATOM	578	C	SER A			-18.838	13.523	1.00 40.66 1.00 40.90	A A
MOTA	579 500		SER A			-19.516 -17.608	12.608 13.341	1.00 40.90	A
atom atom	580 581	N CA	LEU :			-17.608	12.030	1.00 39.32	A
ATOM	582					-15.632	12.082	1.00 38.99	A
ATOM	583					-15.651	11.598	1.00 40.31	A
ATOM	584		1 LEU			-16.860	12.152	1.00 39.79	A
ATOM	585		2 LEU			-14.363	12.024	1.00 40.04	A
MOTA	586		LEU .			-16.778	11.492	1.00 38.55	A
ATOM	587	0	LEU .	A 73	55.028	-16.806	10.280	1.00 36.83	A

ATOM	588	N	ILE 2	A	74	55.780 -	16.576	12.383	1.00 39.70	A
ATOM	589	CA	ILE A		74	57.158 -	16.402	11.942	1.00 41.87	A
ATOM	590	CB	ILE 2	A	74	58.104 -	16.084	13.123	1.00 41.88	A
ATOM	591	CG2	ILE 2	A	74	59.552 -		12.640	1.00 41.29	A
MOTA	592		ILE 2		74	57.729 -		13.738	1.00 41.53	A
MOTA	593		ILE :		74	58.519 -		14.990	1.00 40.94	A
MOTA	594	C	ILE .		74	57.599 -		11.273	1.00 42.04	A A
ATOM	595	0	ILE .		74	58.119 -		10.157	1.00 41.12 1.00 43.51	A
MOTA	596	N	LYS		75	57.364 -		11.954 11.423	1.00 46.61	A
ATOM	597	CA	LYS .		75 75	57.730 - 57.470 -		12.466	1.00 47.84	A
ATOM	598	CB CG	LYS .		75 75	58.096		13.828	1.00 50.82	A
ATOM ATOM	599 600	CD	LYS		75	57.661		14.828	1.00 53.97	A
ATOM	601	CE	LYS		75	58.005		16.269	1.00 55.95	· A
MOTA	602	NZ	LYS		75	59.472		16.531	1.00 56.31	A
ATOM	603	C	LYS		75	56.944	-20.452	10.151	1.00 47.99	A
MOTA	604	0	LYS	A	75	57.530 ·	-20.720	9.106	1.00 48.11	A
ATOM	605	N	ARG	A	76	55.617		10.242	1.00 49.31	A
MOTA	606	CA	arg		76	54.763		9.103	1.00 50.89	A
MOTA	607	CB	ARG		76	53.287		9.530	1.00 53.08	A
ATOM	608	CG	ARG		76	52.960		10.538	1.00 56.83 1.00 58.85	A A
ATOM	609	CD	ARG		76 76	51.478 · 50.620 ·		10.574 11.212	1.00 60.24	A
ATOM	610	NE	ARG		76 76	49.786		10.557	1.00 61.29	A
ATOM	611	CZ	ARG ARG		76 76	49.692		9.234	1.00 60.08	A
ATOM	612 613	NH2			76	49.044		11.226	1.00 61.97	A
ATOM ATOM	614	C	ARG		76	54.947		7.864	1.00 50.93	A
ATOM	615	ŏ	ARG		76	54.705		6.747	1.00 51.19	A
ATOM	616	N	SER		77	55.380		8.046	1.00 50.61	A
ATOM	617	CA	SER		77	55.574	-17.745	6.900	1.00 50.08	A
ATOM	618	CB	SER	A	77	55.262	-16.295	7.282	1.00 50.05	A
MOTA	619	OG	SER	A	77	56.223		8.193	1.00 49.23	A
ATOM	620	C	SER	A	77	57.006		6.386	1.00 49.56	A
ATOM	621	0	ser		77	57.420		5.558	1.00 49.40	A
MOTA	622	N	asn		78		-18.817	6.866	1.00 49.24	A A
ATOM	623	CA	ASN		78		-18.982	6.472	1.00 49.14 1.00 48.86	A
ATOM	624	CB	ASN		78		-19.307 -19.689	4.976 4.558	1.00 48.09	A
MOTA	625	CG	ASN		78 78		-20.442	5.254	1.00 46.05	A
ATOM	626 627		ASN ASN		78		-19.182	3.409	1.00 47.78	A
MOTA MOTA	628	C	ASN		78		-17.667	6.803	1.00 49.08	A
ATOM	629	ō	ASN		78		-17.114	6.001	1.00 48.39	A
MOTA	630	N	SER		79	59.571	-17.177	8.006	1.00 48.58	A
MOTA	631	CA	SER	A	79	60.139	-15.945	8.538	1.00 48.38	A
MOTA	632	CB	SER	A	79		-16.208	9.071	1.00 48.53	A
MOTA	633	OG	SER	A	79		-16.612	8.027	1.00 50.05	A
MOTA	634	С	SER		79		-14.768	7.573	1.00 47.13	A A
MOTA	635	0	SER		79		-14.098	7.444 6.887	1.00 47.66 1.00 45.82	A
MOTA	636	N	THR		80		-14.516 -13.379	5.982	1.00 45.51	A
MOTA	637	CA CB	THR THR		80 80		-13.501	5.016	1.00 47.03	A
MOTA MOTA	638 639	OG:			80		-13.963	5.731	1.00 47.95	A
ATOM	640		2 THR		80		-14.487	3.909	1.00 47.59	A
ATOM	641	C	THR		80	58.855	-12.147	6.882	1.00 44.25	A
MOTA	642		THR		80	57.835	-11.976	7.556	1.00 43.69	A
MOTA	643	N	ALA	. A	81		-11.311	6.903	1.00 41.47	A
ATOM	644	CA	ALA		81		-10.119	7.740	1.00 38.59	A
MOTA	645		ALA		81	61.363	-9.734	8.039	1.00 38.61 1.00 36.89	A A
ATOM	646		ALA		81	59.168	-8.915		1.00 35.83	A
MOTA	647		ALA		81	58.766	-8.884 -7.920		1.00 34.86	A
MOTA	648		ALA		82 82	58.993 58.300			1.00 33.41	A
ATOM ATOM	649 650					57.957			1.00 34.17	A
MOTA	651		ALA			59.141			1.00 32.28	A
MOTA	652		ALA			60.372			1.00 28.62	A
MOTA	653		THE			58.457		5.878		A
ATOM	654					59.100				A
MOTA	655					58.377				A
MOTA	656		1 THE			58.347			_	A A
ATOM	657		2 THE			59.098				A
MOTA	658		THE			59.041				A
MOTA	659		THE			58.029 60.130				A
MOTA MOTA	660 66:					60.188				A
5.4 V.										

3.0004		an .	3 031		0.4	61.634	-0.252	6.069	1.00 36.13	A
MOTA	662	CB	asn		84					
MOTA	663	CG	asn	A	84	62.337	-1.045	7.132	1.00 37.22	A
MOTA	664	OD1	asn	A	84	61.809	-1.241	8.220	1.00 39.34	A
MOTA	665	ND2	ASN	A	84	63.548	-1.497	6.830	1.00 38.89	A
					84	59.549	0.267	4.881	1.00 35.51	A
MOTA	666	C	ASN							A
MOTA	667	0	nra	A	84	59.961	0.343	3.724	1.00 38.89	
MOTA	668	N	GLΰ	A	85	58.546	1.004	5.344	1.00 34.17	A
ATOM	669	CA	GLU	A	85	57.890	2.001	4.507	1.00 32.82	A
			GLU		85	56.427	2.183	4.921	1.00 36.55	A
ATOM	670	CB							1.00 42.74	A
MOTA	671	CG	GLŪ	A	85	55.523	0.993	4.645		
MOTA	672	CD	GLU	A	85	55.271	0.782	3.167	1.00 46.65	A
MOTA	673	OE1	GLU	A	85	54.829	1.741	2.494	1.00 49.22	A
			GLU		85	55.508	-0.345	2.679	1.00 48.74	A
MOTA	674							4.701	1.00 30.10	A
ATOM	675	C	GTA		85	58.624	3.328			
ATOM	676	0	GLU	A	85	59.489	3.453	5.571	1.00 27.29	A
ATOM	677	N	VAL	A	86	58.274	4.308	3.878	1.00 28.67	A
ATOM	678	CA	VAL		86	58.849	5.641	3.951	1.00 27.33	A
						59.146	6.202	2.539	1.00 27.74	A
ATOM	679	CB	VAL		86					
MOTA	680	CG1	VAL	A	86	59.688	7.637	2.640	1.00 22.06	A
ATOM	681	CG2	VAL	A	86	60.139	5.289	1.815	1.00 25.30	A
ATOM	682	C	VAL		86	57.786	6.519	4.614	1.00 27.98	A
							6.671	4.086	1.00 28.76	A
ATOM	683	0	VAL		86	56.685				A
ATOM	684	N	PRO	A	87	58.095	7.098	5.784	1.00 27.39	
ATOM	685	CD	PRO	A	87	59.268	6.861	6.644	1.00 26.00	A
		CA	PRO		87	57.106	7.949	6.458	1.00 28.38	A
ATOM	686						7.989	7.899	1.00 26.97	A
MOTA	687	СВ	PRO		87	57.611				
ATOM	688	CG	PRO	A	87	59.099	7.915	7.727	1.00 27.97	A
ATOM	689	С	PRO	A	87	56.963	9.341	5.848	1.00 30.15	A
	690	ō	PRO		87	57.902	9.871	5.245	1.00 31.62	A
MOTA							9.922	6.004	1.00 29.70	A
MOTA	691	N	GLU		88	55.778				A
ATOM	692	CA	GLU	A	88	55.489	11.252	5.481	1.00 29.65	
ATOM	693	СВ	GLU	A	88	54.173	11.229	4.699	1.00 32.09	A
ATOM	694	CG	GLU	A	88	54.038	12.330	3.655	1.00 38.40	A
						52.790	12.172	2.792	1.00 41.07	A
MOTA	695	æ	ŒΙŪ		88					A
MOTA	696	OE1	GLU	A	88	51.675	12.411	3.303	1.00 42.35	
MOTA	697	OB2	GLU	A	88	52.925	11.800	1.604	1.00 43.46	A
ATOM	698	С	GLU	Δ	88	55.385	12.191	6.680	1.00 27.98	A
						54.588	11.954	7.597	1.00 26.16	A
MOTA	699	0	GLU		88				1.00 23.90	A
ATOM	700	N	VAL	A	89	56.187	13.253	6.672		
ATOM	701	CA	VAL	A	89	56.201	14.194	7.788	1.00 21.62	A
ATOM	702	CB	VAL	A	89	57.637	14.358	8.333	1.00 18.36	A
			. VAL		89	57.639	15.295	9.534	1.00 17.11	A
MOTA	703							8.719	1.00 16.77	A
ATOM	704	CG2	. VAL		89	58.204	12.990			
MOTA	705	C	VAL	Α	89	55.626	15.575	7.483	1.00 21.60	A
MOTA	706	0	VAL	A	89	55.859	16.143	6.420	1.00 21.72	A
MOTA	707	N	THR		90	54.886	16.115	8.444	1.00 21.28	A
						54,269	17.425	8.301	1.00 20.62	A
MOTA	708	CA	THR		90					A
MOTA	709	CB	THR	A	90	52.813	17.303	7.823	1.00 21.90	
ATOM	710	OG:	LTHR	A	90	52.770	16.537	6.613	1.00 26.43	A
ATOM	711	CG	THR	. A	90	52.220	18.678	7.558	1.00 23.70	A
		C.	THR		90	54.264	18.153	9.639	1.00 21.08	A
MOTA	712								1.00 20.41	A
ATOM	713	0	THE		90	53.887	17.578	10.667		
ATOM	714	N	VAL	A	91	54.670	19.423	9.618	1.00 19.24	A
ATOM	715	CA	VAI	A	91	54.712	20.243	10.822	1.00 19.55	A
	716		VAI		91	56.149	20.739	11.102	1.00 19.97	A
MOTA						56.167	21.629	12.338	1.00 16.82	A
MOTA	717		l VAI							A
MOTA	718	CG	2 VAI	ιA	91	57.072	19.547	11.280	1.00 17.43	
MOTA	719	C	VAI	À	91	53.789	21.452	10.703	1.00 19.10	A
ATOM	720		VAI	A	91	53.735	22.108	9.666	1.00 20.59	A
			PHE			53.059	21,739	11.772	1.00 18.65	A
ATOM	721						22.870	11.785	1.00 19.10	A
MOTA	722	CA				52.146				
MOTA	723	CB	PHI	A E	. 92	50.853	22.516	11.030	1.00 18.89	A
MOTA	724	CG	PHI	B A	92	50.176	21,264	11.525	1.00 16.16	A
ATOM	725		1 PH			49.165		12.480	1.00 16.77	A
						50.561		11.047	1.00 16.62	A
MOTA	726		2 PHI							A
ATOM	727	CE	1 PH	g A	. 92	48.543		12.955		
ATOM	728	CE	2 PH	EΑ	92	49.954	18.848	11.511	1.00 18.17	A
ATOM	729			e A		48.936	18.922	12.471	1.00 17.05	A
				E A		51.844		13.229		A
ATOM	730							14.134		A
MOTA	731			E A		52.055				
ATOM	732	N	SE	R A	93	51.365		13.445		A
ATOM	733			R A		51.052	24.896	14.792	1.00 19.26	A
ATOM				R A		51.275		14.921		A
	734					50.435		14.043		A
MOTA	735	S OG	: SE	R A	93	50.435	61.132	74.043	2.00 20.27	7-

ATOM	736	С	SER A	93	49.618	24.554	15.172	1.00 19.04	A
ATOM	737	ō	SER A	93	48.748	24.417	14.316	1.00 17.44	A
ATOM	738	N	LYS A	94	49.390	24.418	16.472	1.00 20.26	A
ATOM	739	CA	LYS A	94	48.077	24.108	17.010	1.00 21.70	A
ATOM	740	CB	LYS A	94	48.227	23.670	18.464	1.00 22.45	A
ATOM	741	CG	LYS A	94	46.938	23.273	19.139	1.00 24.42	A
		CD	LYS A	94	47.189	22.867	20.587	1.00 25.48	A
MOTA MOTA	742 743	CE	LYS A	94	45.881	22.548	21.297	1.00 25.73	A
		NZ	LYS A	94	45.122	21.533	20.517	1.00 26.34	A
ATOM	744 745	C	LYS A	94	47.169	25.340	16.921	1.00 23.44	A
MOTA MOTA	746	ō	LYS A	94	45.984	25.235	16.598	1.00 20.95	A
	747	И	SER A	95	47.742	26.505	17.212	1.00 24.82	A
MOTA	748	CA	SER A	95	47.013	27.769	17.172	1.00 27.69	A
MOTA MOTA	749	CB	SER A	95	46.969	28.408	18.565	1.00 26.33	Α.
ATOM	750	og	SER A	95	46.202	27.635	19.468	1.00 32.56	A
ATOM	751	C	SER A	95	47.688	28.747	16.219	1.00 27.36	A
MOTA	752	ŏ	SER A	95	48.824	28.529	15.797	1.00 27.94	A
MOTA	753	и	PRO A	96	46.985	29.830	15.849	1.00 27.27	A
MOTA	754	CD CD	PRO A	96	45.611	30.232	16.193	1.00 28.85	A
ATOM	755	CA	PRO A	96	47.606	30.801	14.946	1.00 26.90	A
MOTA	756	СВ	PRO A	96	46.471	31.788	14.663	1.00 28.13	A
ATOM	757	CG	PRO A	96	45.634	31.719	15.907	1.00 28.36	A
ATOM	758	C	PRO A	96	48.786	31.421	15.700	1.00 24.92	A
ATOM	759	ō	PRO A	96	48.757	31.556	16.925	1.00 24.65	A
ATOM	760	N	VAL A	97	49.828	31.786	14.973	1.00 24.24	A
ATOM	761	CA	VAL A	97	51.016	32.332	15.601	1.00 25.15	A
ATOM	762	СВ	VAL A	97	52.261	32.087	14.715	1.00 26.78	A
ATOM	763		VAL A	97	53.531	32.372	15.508	1.00 26.15	A
ATOM	764		VAL A		52.255	30.659	14.198	1.00 26.15	A
ATOM	765	C	VAL A		50.935	33.820	15.920	1.00 25.62	A
ATOM	766	0	VAL A		50.624	34.638	15.054	1.00 25.01	A
ATOM	767	N	THR A		51.207	34.157	17.175	1.00 24.46	A
ATOM	768	CA	THR A	98	51.212	35.542	17.627	1.00 25.36	A
ATOM	769	CB	THR A	98	49.835	35.941	18.283	1.00 25.29	A
ATOM	770	OG1	THR A	. 98	50.030	37.008	19.217	1.00 30.50	A
MOTA	771	CG2	THR A	98	49.196	34.771	18.985	1.00 29.80	A
ATOM	772	C	THR A	. 98	52.382	35.678	18.605	1.00 24.87	A
ATOM	773	0	THR A	. 98	52.499	34.902	19.554	1.00 23.01	A
MOTA	774	N	LEU A	99	53.273	36.634	18.344	1.00 25.94	A
ATOM	775	CA	LEU A	. 99	54.445	36.843	19.198	1.00 28.02	A
MOTA	776	CB	LEU A	99	55.194	38.114	18.797	1.00 31.12	A
MOTA	777	CG	TER Y	. 99	55.950	38.211	17.469	1.00 35.44	A
ATOM	778	CD1	LEU A	. 99	56.650	39.577	17.416	1.00 35.45	A
MOTA	779	CD2	LEU A		56.970	37.087	17.341	1.00 35.62	A
MOTA	780	С	LEU A		54.135	36.932	20.689	1.00 27.10	A
MOTA	781	0	LEU A		53.201	37.616	21.097	1.00 25.34	A
ATOM	782	N	GLY A		54.935	36.233	21.492	1.00 26.71	A
ATOM	783	CA	GLY A		54.762	36.253	22.935	1.00 26.48	A
MOTA	784	С	GLY A		53.635	35.398	23.479	1.00 26.32	A
MOTA	785	0	GLY A		53.428	35.323	24.695	1.00 25.37	A
MOTA	786	N	GLN A		52.913	34.734	22.585	1.00 25.16	A A
MOTA	787	CA	GLN A		51.796	33.896	22.999 22.143	1.00 25.74 1.00 28.06	A
MOTA	788	CB	GLN A		50.573	34.219	22.143	1.00 20.50	A
ATOM	789	CG	GLN A		49.258 49.123	33.911 34.599	24.162	1.00 32.88	A
ATOM	790	CD	CILN 3		48.953	35.820	24.251	1.00 30.83	A
MOTA	791		GPN 1		49.202	33.813	25.221	1.00 33.04	A
MOTA	792		GLN I		52.117	32.409	22.901	1.00 24.01	A
MOTA	793	C	GLN A		52.280	31.881	21.807	1.00 24.25	A
ATOM ATOM	794 795	И	PRO I		52.199	31.715	24.051	1.00 22.08	A
MOTA	796	CD	PRO A		51.959	32.244	25.410	1.00 22.41	A
MOTA	797	CA	PRO I		52.500	30.278	24.096	1.00 21.37	A
MOTA	798	CB	PRO I		52.136	29.898	25.526	1.00 21.61	A
ATOM	799	œ	PRO I		52.521	31.147	26.297	1.00 21.90	A
ATOM	800	C		A 102	51.706	29.480	23.068	1.00 21.30	A
ATOM	801	Ö		A 102	50.496	29.644	22.947	1.00 21.93	A
MOTA	802			A 103	52.396	28.618	22.327	1.00 18.86	A
ATOM	803	CA		A 103	51.749	27.802	21.305	1.00 17.69	A
ATOM	804	CB		A 103	52.040	28.379	19.913	1.00 17.99	A
MOTA	805			A 103	50.899	28.162	18.929		A
MOTA	806		1 ASN		50.348	27.060	18.808	1.00 17.82	A
MOTA	807		2 ASN		50.549	29.223	18.204	1.00 17.71	A
ATOM	808			A 103	52.281	26.370	21.385	1.00 15.57	A
MOTA	809	0	ASN .	A 103	53.000	26.012	22.310	1.00 14.67	A

ATOM	810	N	ILE A 104	51.918	25.565	20.397	1.00 15.80	A
MOTA	811	CA CB	ILE A 104 ILE A 104	52.335 51.255	24.177 23.235	20.328	1.00 13.66	A A
MOTA MOTA	812 813		ILE A 104	51.589	21.792	20.539	1.00 13.40	A
ATOM	814		ILE A 104	51.132	23.421	22.400	1.00 17.40	A
MOTA	815	CD1	ILE A 104	50.129	22.494	23.047	1.00 18.65	A
MOTA	816	C	ILE A 104	52.588	23.775	18.896	1.00 14.36	A
MOTA	817	0	ILE A 104	51.716	23.924	18.052	1.00 16.86	A
MOTA MOTA	818 819	N CA	LEU A 105 LEU A 105	53.785 54.090	23.272 22.822	18.616 17.272	1.00 15.67 1.00 15.52	A A
ATOM	820	СВ	LEU A 105	55.568	22.978	16.940	1.00 15.73	A
ATOM	821	CG	LEU A 105	56.058	24.391	16.649	1.00 20.75	A
MOTA	822		LEU A 105	57.400	24.298	15.919	1.00 20.19	A
MOTA	823	-	LEU A 105	55.030	25.141	15.791	1.00 21.31	A
ATOM	824	C	LEU A 105 LEU A 105	53.709 53.968	21.362 20.589	17.202 18.133	1.00 15.97 1.00 14.11	A A
ATOM ATOM	825 826	O N	ILB A 106	53.078	20.993	16.099	1.00 14.18	A
ATOM	827	CA	ILE A 106	52.643	19.630	15.903	1.00 15.40	A
ATOM	828	CB	ILE A 106	51.122	19.576	15.636	1.00 15.11	A
MOTA	829		ILE A 106	50.661	18.135	15.592	1.00 12.46	A
ATOM	830		ILE A 106	50.380	20.354	16.734	1.00 15.51 1.00 12.83	A A
ATOM ATOM	831 832	CDI	ILE A 106 ILE A 106	48.862 53.381	20.413 19.011	16.565 14.725	1.00 16.48	A
MOTA	833	ō	ILE A 106	53.484	19.607	13.651	1.00 17.37	A
ATOM	834	N	CYS A 107	53.900	17.811	14.944	1.00 17.86	A
MOTA	835	CA	CYS A 107	54.621	17.083	13.917	1.00 18.32	A
MOTA	836	C	CYS A 107	53.886	15.776	13.663	1.00 18.29	A
MOTA	837	0	CYS A 107	53.846 56.041	14.909 16.792	14.533 14.382	1.00 18.13 1.00 19.33	A A
MOTA MOTA	838 839	CB SG	CYS A 107 CYS A 107	57.029	15.889	13.158	1.00 25.82	A
ATOM	840	N	LEU A 108	53.304	15.649	12.472	1.00 17.89	A
ATOM	841	CA	LEU A 108	52.556	14.456	12.088	1.00 18.82	A
MOTA	842	CB.	LEU A 108	51.330	14.850	11.252	1.00 20.17	A
MOTA	843	CG	LEU A 108	50.129	13.900	11.053 9.624	1.00 21.48 1.00 20.62	A A
MOTA	844 845		LEU A 108	49.623 50.493	14.049 12.458	11.316	1.00 18.40	A
ATOM	846	C	LEU A 108	.53.445	13.538	11.252	1.00 19.49	A
ATOM	847	o	LEU A 108	53.841	13.892	10.144	1.00 20.39	A
ATOM	848	N	VAL A 109	53.760	12.368	11.789	1.00 18.45	A
ATOM	849	CA	VAL A 109	54.586	11.398	11.087	1.00 19.04	A A
ATOM	850	CB	VAL A 109 VAL A 109	55.665 56.626	10.805 9.923	12.042 11.279	1.00 18.71 1.00 15.16	A
ATOM ATOM	851 852		VAL A 109	56.431	11.949	12.729	1.00 17.68	A
ATOM	853	C	VAL A 109	53.611	10.322	10.606	1.00 20.50	A
MOTA	854	0	VAL A 109	53.115	9.516	11.393	1.00 21.55	A
MOTA	855	N	ASP A 110	53.326	10.337	9.308	1.00 21.50	A
MOTA	856	CA	ASP A 110 ASP A 110	52.376 51.493	9.407 10.165	8.700 7.701	1.00 21.95 1.00 22.25	A A
MOTA MOTA	857 858	CB CG	ASP A 110	50.084	9.612	7.622	1.00 24.20	A
ATOM	859		ASP A 110	49.874	B.435	7.989	1.00 23.87	A
MOTA	860	OD2	ASP A 110	49.182	10.356	7.182	1.00 25.94	A
MOTA	861	C	ASP A 110	53.059	8.240	7.985	1.00 21.53	A.
MOTA MOTA	862	0	ASP A 110 ASN A 111	54.273 52.254	8.254 7.245	7.782 7.603	1.00 23.78	A A
ATOM	863 864	N CA	ASN A 111	52.706	6.037	6.900	1.00 23.32	A
ATOM	865	СВ	ASN A 111	53.046	6.360	5.437	1.00 24.67	A
MOTA	866	CG	ASN A 111	53.181	5.102	4.575	1.00 31.76	A
MOTA	867		L ASN A 111	52.291	4.240	4.567	1.00 31.05 1.00 29.09	A A
MOTA	868		ASN A 111 ASN A 111	54.292 53.905	4.994 5.389	3.842 7.587	1.00 23.68	A
MOTA MOTA	869 870	C	ASN A 111	54.953	5.156	6.976	1.00 22.88	A
ATOM	871	N	ILE A 112	53.738	5.090	8.868	1.00 22.97	A
ATOM	872	CA	ILE A 112	54.797	4.473	9.646	1.00 20.73	A
MOTA	873	CB	ILE A 112	54.791	4.967	11.108	1.00 20.13 1.00 15.53	A A
MOTA	874		2 ILE A 112	55.979 54.833	4.363 6.495	11.864 11.158	1.00 15.53	A
MOTA MOTA	875 876		1 ILE A 112 1 ILE A 112	54.671		12.575		A
MOTA	877	CD.	ILE A 112	54.658	2.960	9.699	1.00 22.54	A
ATOM	878	ō	ILE A 112	53.605	2.436		1.00 22.65	A
MOTA	879	N	PHE A 113	55.732				A A
ATOM	880	CA		55.769 54 742				A A
MOTA MOTA	881 882		PHE A 113	54.742 54.451				A
ATOM	883		1 PHE A 113	53.528				A

ATOM	884	സാ	PHE A	112	55.183	-2.296	8.285	1.00 20.76	A
ATOM	885		PHE A		53.341	-2.848	10.302	1.00 19.85	A
			PHE A		55.008	-3.607	8.721	1.00 20.75	A
ATOM	886					-3.887			
ATOM	887	CZ	PHE A		54.086		9.735	1.00 21.24	A
ATOM	888	C	PHE A		57.157	0.329	9.042	1.00 21.21	A
ATOM	889	0	PHE A		57.700	0.719	8.011	1.00 19.97	A
ATOM	890	N	PRO A		57.765	-0.509	9.893	1.00 22.22	A
ATOM	891	ÇD.	PRO A		59.118	-1.018	9.614	1.00 22.88	A
MOTA	892	CA	PRO A		57.263	-1.040	11.170	1.00 23.38	A
ATOM	893	CB	PRO A		58.340	-2.045	11.571	1.00 23.68	A
ATOM	894	CG	PRO A	114	59.592	-1.435	10.984	1.00 23.26	A
MOTA	895	C	PRO A	114	57.078	0.059	12.221	1.00 24.33	A
ATOM	896	0	PRO A	114	57.571	1.174	12.054	1.00 24.35	A
ATOM	897	N	PRO A	115	56.363	-0.247	13.319	1.00 24.59	A
ATOM	898	CD	PRO A	115	55.579	-1.472	13.567	1.00 22.60	A
MOTA	899	CA	PRO A	115	56.135	0.751	14.372	1.00 23.79	A
MOTA	900	CB	PRO A	115	54.923	0.194	15,107	1.00 23.96	A
MOTA	901	CG	PRO A	115	55.129	-1.291	14.998	1.00 23.45	A
ATOM	902	С	PRO A		57.337	0.996	15.289	1.00 24.97	A
ATOM	903	0	PRO A		57.322	0.670	16.482	1.00 23.11	A
ATOM	904	N	VAL A		58.380	1.573	14.705	1.00 24.77	A
ATOM	905	CA	VAL A		59.607	1.902	15.423	1.00 24.05	A
ATOM	906	CB	VAL A		60.733	0.881	15.135	1.00 26.45	A
ATOM	907		VAL A		61.977	1.250	15.933	1.00 24.89	A
			VAL A		60.267	-0.539	15.470	1.00 26.43	A
MOTA	908						14.875	1.00 24.47	À
MOTA	909	C	VAL A		60.043	3.254			A
ATOM	910	0	VAL A		60.340	3.381	13.684	1.00 23.94 1.00 22.43	
MOTA	911	N	VAL A		60.088	4.269	15.728		A
ATOM	912	CA	VAL A		60.472	5.577	15.239	1.00 22.18	A
MOTA	913	CB	VAL A		59.247	6.277	14.565	1.00 21.24	A
ATOM	914		VAL A		58.276	6.807	15.631	1.00 17.87	A
ATOM	915	CG2	VAL A		59.710	7.387	13.653	1.00 19.98	A
ATOM	916	C	VAL A		61.035	6.484	16.326	1.00 23.40	A
ATOM	917	ο.	VAL A	117	60.743	6.323	17.512	1.00 22.77	A
MOTA	918	N	ASN A	118	61.868	7.427	15.909	1.00 24.87	A
MOTA	919	CA	ASN A	118	62.434	8.398	16.833	1.00 25.96	A
MOTA	920	CB	ASN A	118	63.970	8.341	16.858	1.00 29.36	A
ATOM	921	CG	ASN A	. 118	64.506	7.213	17.728	1.00 31.24	A
ATOM	922	OD1	ASN A	. 118	63.885	6.833	18.722	1.00 34.20	A
MOTA	923	ND2	ASN A	. 118	65.679	6.694	17.374	1.00 34.04	A
ATOM	924	C	ASN A	. 118	61.989	9.746	16.312	1.00 24.87	A
ATOM	925	0	ASN A	. 118	62.298	10.112	15.177	1.00 26.17	A
MOTA	926	N	ILE A		61.229	10.468	17.122	1.00 23.82	A
MOTA	927	CA	ILE A		60.774	11.793	16.727	1.00 23.07	A
MOTA	928	СВ	ILE A		59.231	11.892	16.711	1.00 22.65	A
ATOM	929		ILE A		58.797	13.197	16.051	1.00 18.01	A
ATOM	930		ILE A		58.642	10.716	15.936	1.00 21.02	A
ATOM	931		ILE A		57.135	10.714	15.921	1.00 21.88	A
	932	c	ILE A		61.323	12.771	17.754	1.00 22.76	A
MOTA		0	ILE A		61.013	12.680	18.940	1.00 22.92	A
MOTA	933				62.162	13.691	17.303	1.00 23.11	A
ATOM	934	N	THR A				18.205	1.00 23.65	A
ATOM	935	CA	THR A		62.737	14.673			A
MOTA	936	CB	THR A		64.216	14.363	18.495	1.00 25.23	
ATOM	937		THR A		64.921	14.199	17.258	1.00 26.55	A
ATOM	938		THR A		64.335	13.081	19.331	1.00 23.93	A
MOTA	939	С	THR A		62.622	16.064	17.616	1.00 23.20	A
MOTA	940	0	THR A		62.437	16.232	16.412	1.00 23.15	A
MOTA	941	N	TRP A		62.725	17.069	18.470	1.00 22.54	A
MOTA	942	CA	TRP A		62.619	18.432	17.998	1.00 21.37	A
MOTA	943	CB	TRP A		61.563	19.196	18.791	1.00 19.43	A
MOTA	944	CG	TRP A		60.173	18.679	18.616	1.00 18.76	A
ATOM	945	CD2	TRP A	121	59.191	19.179	17.703	1.00 19.96	A
ATOM	946	CE2	TRP A	121	58.002	18.454	17.931	1.00 18.06	A
ATOM	947	CE3	TRP A	121	59.200	20.178	16.715	1.00 16.07	A
ATOM	948		TRP A		59.567	17.694	19.330	1.00 18.18	A
ATOM	949		TRP F		58.261	17.553	18.929	1.00 19.21	A
MOTA	950		TRP #		56.827	18.694	17.210	1.00 16.20	A
ATOM	951		TRP A		58.036	20.419	16.000	1.00 16.43	A
ATOM	952		TRP I		56.864	19.679	16.252	1.00 17.37	A
MOTA	953	C	TRP A		63.927	19.178	18.097	1.00 22.88	A
ATOM	954	ō	TRP A		64.743	18.937	18.992	1.00 22.75	A
MOTA	955	N	LEU A		64.109	20.100	17.164	1.00 23.24	A
ATOM	956	CA	LEU A		65.291	20.930	17.136	1.00 22.66	A
MOTA	957	CB	LEU 1		66.094	20.699	15.850	1.00 23.05	A
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ATOM	958	CG	LEU A 122	66.638	19.293	15.563	1.00 22.23	A
ATOM	959		LEU A 122	67.404	19.326	14.253	1.00 20.93	A
MOTA MOTA	960 961	CD2	LEU A 122 LEU A 122	67.542 64.837	18.830 22.376	16.700 17.186	1.00 20.21 1.00 23.52	A A
ATOM	962	ō	LEU A 122	63.830	22.752	16,572	1.00 21.74	A
ATOM	963	N	SER A 123	65.579	23.174	17.945	1.00 23.69	A
ATOM	964	CA	SER A 123	65.330	24.597	18.063	1.00 24.10 1.00 25.22	A
ATOM ATOM	965 966	CB OG	SER A 123 SER A 123	64.998 64.735	24.983 26.373	19.504 19.591	1.00 25.22	A A
ATOM	967	C	SER A 123	66.664	25.200	17.650	1.00 24.79	A
ATOM	968	0	SER A 123	67.670	25.014	18.335	1.00 23.07	A
MOTA	969	N	ASN A 124	66.666	25.903	16.521	1.00 25.02	A
ATOM	970 971	CA CB	ASN A 124 ASN A 124	67.880 68.351	26.513 27.676	15.986 16.868	1.00 25.63 1.00 24.46	A A
ATOM ATOM	972	CG	ASN A 124	67.376	28.839	16.873	1.00 25.33	A
ATOM	973		ASN A 124	66.636	29.056	15.907	1.00 26.04	A
ATOM	974		ASN A 124	67.381	29.606	17.956	1.00 21.77	A
ATOM	975 976	C 0	ASN A 124 ASN A 124	69.006 70.132	25.487 25.706	15.838 16.301	1.00 26.53 1.00 26.36	A A
MOTA MOTA	977	И	GLY A 125	68.684	24.361	15.205	1.00 24.78	A
ATOM	978	CA	GLY A 125	69.669	23.326	14.964	1.00 26.09	A
MOTA	979	C	GLY A 125	70.030	22.377	16.089	1.00 27.35	A
MOTA	980	0	GLY A 125 HIS A 126	70.728 69.566	21.395 22.645	15.846 17.307	1.00 28.21 1.00 28.65	A A
ATOM ATOM	981 982	N CA	HIS A 126	69.889	21.774	18.430	1.00 30.12	A
ATOM	983	СВ	HIS A 126	70.816	22.507	19.408	1.00 32.68	A
MOTA	984	CG	HIS A 126	70.226	23.750	19.996	1.00 35.25	A
MOTA	985		HIS A 126	70.296 69.475	25.044	19.601 21.151	1.00 36.90 1.00 35.93	A A
ATOM ATOM	986 987		HIS A 126 HIS A 126	69.110	23.743 24.979	21.445	1.00 36.88	A
ATOM	988		HIS A 126	69.595	25.788	20.520	1.00 36.73	A
MOTA	989	C	HIS A 126	68.661	21.220	19.149	1.00 30.87	A
ATOM	990	0	HIS A 126	67.634	21.889	19.270	1.00 31.49	A A
ATOM ATOM	991 992	n Ca	SER A 127 SER A 127	68.789 67.697	19.990 19.286	19.635 20.302	1.00 30.93 1.00 33.08	A
ATOM	993	СВ	SER A 127	68.165	17.889	20.714	1.00 33.91	A
ATOM	994	OG	SER A 127	69.231	17.979	21.645	1.00 38.34	A
ATOM	995	C	SER A 127	67.050	19.971	21.501	1.00 32.98	A A
MOTA MOTA	996 997	N O	SER A 127 VAL A 128	67.708 65.743	20.654 19.770	22.288 21.624	1.00 34.83 1.00 32.42	Ā
ATOM	998	CA	VAL A 128	64.960	20.325	22.716	1.00 31.29	A
MOTA	999	CB	VAL A 128	63.645	20.921	22.202	1.00 30.48	A
MOTA	1000		VAL A 128	62.856	21.520	23.358	1.00 27.06	A
ATOM	1001		VAL A 128 VAL A 128	63.937 64.645	21.970 19.183	21.142 23.669	1.00 28.52 1.00 32.28	A A
MOTA MOTA	1002 1003	0	VAL A 128	64.275	18.093	23.237	1.00 32.80	A
ATOM	1004	N	THR A 129	64.786	19.437	24.965	1.00 33.30	A
MOTA	1005	CA	THR A 129	64.546	18.411	25.981	1.00 33.70	A
MOTA	1006	CB OG1	THR A 129 THR A 129	65.740 65.969	18.344 19.643	26.966 27.528	1.00 34.52 1.00 38.18	A A
ATOM ATOM	1007 1008	CG2		67.006	17.898	26.245	1.00 34.60	A
MOTA	1009	Ç	THR A 129	63.257	18.591	26.791	1.00 32.08	A
MOTA	1010	0	THR A 129	62.645	17.615	27.220	1.00 34.04	A
MOTA	1011	N	GLU A 130 GLU A 130	62.843 61.639	19.835 20.119	26.993 27.762	1.00 28.85 1.00 26.09	A A
MOTA MOTA	1012 1013	CA CB	GLU A 130	61.926	21.236	28.770	1.00 28.58	A
ATOM	1014	CG	GLU A 130	62.962	20.894	29.822	1.00 32.87	A
ATOM	1015	CD	GLU A 130	62.592	19.654	30.609	1.00 35.34	A
ATOM	1016		GLU A 130	61.392	19.475	30.907 30.941	1.00 37.85 1.00 36.29	A A
ATOM ATOM	1017 1018	C OR	GLU A 130 GLU A 130	63.501 60.451	18.865 20.534	26.893	1.00 23.53	A
ATOM	1019	Ö	GLU A 130	60.629	21.166	25.859	1.00 19.76	A
MOTA	1020	N	GLY A 131	59.243	20.188	27.334	1.00 21.13	A
MOTA	1021	CA	GLY A 131	58.046	20.563	26.601	1.00 20.14 1.00 20.64	A A
MOTA	1022 1023	C	GLY A 131 GLY A 131	57.693 56.989	19.684 20.109	25.421 24.507	1.00 20.11	A
MOTA MOTA	1023	N	VAL A 132	58.164			1.00 18.28	A
MOTA	1025	CA	VAL A 132	57.899	17.527	24.355	1.00 20.08	A
MOTA	1026	CB	VAL A 132	59.230			1.00 20.35	A A
MOTA	1027 1028		1 VAL A 132 2 VAL A 132	58.946 60.006			1.00 22.11	A
MOTA MOTA	1028	C.	VAL A 132	57.027			1.00 20.06	A
ATOM	1030	ō	VAL A 132	57.194	15.794	25.875	1.00 18.65	A
ATOM	1031	N	SER A 133	56.094	15.948	23.925	1.00 17.90	A

MOTA	1032	CA	SER A 133	55.238	14.802	24.215	1.00 18.16	A
ATOM	1033	СВ	SER A 133	54.045	15.206	25.094	1.00 18.24	A
ATOM	1034	og	SER A 133 SER A 133	53.202 54.738	16.143 14.200	24.440 22.914	1.00 24.24 1.00 16.52	A A
MOTA MOTA	1035 1036	0	SER A 133	54.876	14.794	21.843	1.00 16.18	A
ATOM	1037	N	GLU A 134	54.166	13.009	22.996	1.00 17.45	A
ATOM	1038	CA	GLU A 134	53.653	12.369	21.800	1.00 18.50	A
MOTA	1039	CB	GLU A 134	54.797	11.661	21.050	1.00 22.31	A
MOTA	1040	CG	GLU A 134	55.475	10.513	21.801	1.00 24.62	A
ATOM	1041	CD	GLU A 134	56.610	9.859 8.680	20.992 21.254	1.00 28.65 1.00 29.58	A A
MOTA MOTA	1042 1043		GLU A 134 GLU A 134	56.932 57.188	10.521	20.099	1.00 27.96	A
ATOM	1044	C	GLU A 134	52.523	11.389	22.087	1.00 18.44	A
ATOM	1045	ō	GLU A 134	52.279	11.003	23.234	1.00 17.30	A
MOTA	1046	N	THR A 135	51.824	11.008	21.027	1.00 16.71	A
ATOM	1047	CA	THR A 135	50.733	10.059	21.119	1.00 15.49 1.00 16.16	A A
ATOM	1048	CB	THR A 135 THR A 135	49.738 50.369	9.867	19.967 18.731	1.00 16.02	A
ATOM ATOM	1049 1050		THR A 135	49.280	11.697	19.879	1.00 14.19	A
MOTA	1051	c	THR A 135	51.346	8.682	20.946	1.00 17.19	A
ATOM	1052	0	THR A 135	52.551	8.554	20.733	1.00 17.26	A
ATOM	1053	N	SER A 136	50.519	7.650	21.047	1.00 17.53	A
MOTA	1054	CA	SER A 136	51.001	6.297	20.818	1.00 15.92 1.00 16.85	A A
MOTA	1055	CB	SER A 136 SER A 136	50.035 49.756	5.266 5.532	21.416 22.781	1.00 18.22	A
MOTA MOTA	1056 1057	OG C	SER A 136	50.967	6.187	19.294		A
ATOM	1058	ō	SER A 136	50.715	7.169	18.596	1.00 17.25	A
ATOM	1059	N	PHE A 137	51.236	5.003	18.767	1.00 17.08	A
MOTA	1060	CA	PHE A 137	51.155	4.806	17.333	1.00 15.67	A
MOTA	1061	CB	PHE A 137	51.874	3.519	16.936	1.00 13.47	A A
ATOM	1062	CG	PHE A 137 PHE A 137	53.363 54.037	3.628 4.255	16.951 15.907	1.00 15.82	A
ATOM ATOM	1063 1064		PHE A 137	54.100	3.112	18.010	1.00 15.21	A
MOTA	1065		PHE A 137	55.427	4.367	15.918	1.00 15.72	A
MOTA	1066		PHE A 137	55.490	3.220	18.031	1.00 15.14	A
ATOM	1067	CZ	PHE A 137	56.152	3.848	16.983	1.00 14.35	A
ATOM	1068	C	PHE A 137	49.659	4.657 3.767	17.067 17.622	1.00 16.21 1.00 18.05	A A
MOTA	1069	N O	PHE A 137 LEU A 138	49.037 49.074	5.534	16.259	1.00 17.51	A
MOTA MOTA	1070 1071	CA	LEU A 138	47.648	5.433	15.953	1.00 19.20	A
ATOM	1072	CB	LEU A 138	47.017	6.822	15.800	1.00 20.80	A
MOTA	1073	CG	LEU A 138	46.809	7.688	17.044	1.00 23.47	A
MOTA	1074		LEU A 138	46.141	6.879	18.144	1.00 24.75 1.00 27.62	A A
MOTA	1075		LEU A 138	48.140 47.490	8.212 4.637	17.529 14.658	1.00 27.02	A
MOTA MOTA	1076 1077	C	LEU A 138	48.218	4.862	13.698	1.00 16.16	A
MOTA	1078	N	SER A 139	46.530	3.716	14.630	1.00 18.51	A
ATOM	1079	CA	SER A 139	46.333	2.863	13.460	1.00 17.61	A
MOTA	1080	СВ	SER A 139	45.481	1.656	13.836	1.00 18.17	A
ATOM	1081	OG	SER A 139	44.134	2.036	14.040 12.216	1.00 20.80 1.00 17.44	A A
ATOM	1082	0	SER A 139 SER A 139	45.729 45.122	3.510 4.578	12.276	1.00 16.41	A
ATOM ATOM	1083 1084	71	LYS A 140	45.908	2.822	11.088	1.00 18.56	A
ATOM	1085	CA	LYS A 140	45.402	3.237	9.778	1.00 18.37	A
MOTA	1086	CB	LYS A 140	46.543	3.751	8.895	1.00 21.60	A
MOTA	1087	CG	LYS A 140	47.149	5.085	9.326	1.00 24.86 1.00 30.27	A A
ATOM	1088	CD	LYS A 140	46.513 46.961	6.267 6.345	8.602 7.150	1.00 30.27	A
MOTA MOTA	1089 1090	CE NZ	LYS A 140 LYS A 140	48.440		7.038	1.00 30.14	A
ATOM	1091	C	LYS A 140	44.773		9.118	1.00 17.79	A
ATOM	1092		LYS A 140	45.106	0.878	9.458		A
MOTA	1093		SER A 141	43.882		8.160		A
MOTA	1094			43.220		7.481 6.630		A A
MOTA	1095			42.047 42.490				A
ATOM ATOM	1096 1097		SER A 141	44.154				A
ATOM	1098		SER A 141	43.828		6.332	1.00 21.49	A
ATOM	1099		ASP A 142	45.311				A
ATOM	1100			46.234				A A
MOTA	1101			47.008 47.949				A
MOTA MOTA	1102 1103		1 ASP A 142	47.837				A
MOTA	1104		2 ASP A 142	48.799		4.354	1.00 28.43	A
MOTA	1105		ASP A 142	47.176	-0.752	6.368	1.00 20.11	A

MOTA	1106	0	asp			48.		-1.			946	1.00			A
MOTA	1107		HIS			46.		-0.			659 706	1.00			A A
ATOM	1108	CA CB	HIS HIS			47. 47.		-1. -2.			409	1.00			A
ATOM ATOM	1109 1110	CG	HIS			46.		-3.			190	1.00			A
ATOM	1111		HIS			45.		-4.	211	7.	213	1.00	1	7.59	A
ATOM	1112		HIS			45.			151		032			5.97	A
ATOM	1113		HIS				194		786		580			9.46	A A
MOTA	1114		HIS HIS				529 019		436 749		478 030			8.06 9.46	A
ATOM ATOM	1115 1116	C O	HIS				812		401		715			9.95	A
ATOM	1117	N	SER				301	Ο.	454	8.	536	1.00	1	9.70	A
MOTA	1118	CA	SER	A:	144		542		141		852			0.18	A
MOTA	1119	CB	SER				018		011		678 364			.9.91 .3.64	A A
ATOM	1120 1121	OG	SER SER				099 109		044 018	10.				9.40	A
ATOM ATOM	1122	C 0	SER				970		906		499			9.70	A
ATOM	1123	N	PHE				986	2.	883	10.	525			6.99	A
ATOM	1124	CA	PHE	A	145		614		728		649			16.06	A
MOTA	1125	CB	PHE				325		274		929			l6.25 L9.53	A A
ATOM	1126	CG	PHE				.062 .754		841 807		297 672			20.17	A
ATOM ATOM	1127 1128		PHE				114		522		263			18.18	A
ATOM	1129		PHE				505		525	13.	005	1.00	2	21.33	A
ATOM	1130	CE2				49	. 856	0.	193		606			19.50	A
MOTA	1131	CZ	PHE				. 553		.831 .		975			20.23	A
ATOM	1132	C	PHE				.955		.182 .538		419			15.69 16.69	A A
ATOM	1133 1134	N O	PHE				.548 .530		.021		357			14.53	A
MOTA MOTA	1134	CA	PHE				.869		429		332			16.67	A
ATOM	1136	CB	PHE			49	.841	8	. 279	11.	552			16.59	A
MOTA	1137	CG			146		. 535		.528		259			15.25	A
MOTA	1138		PHB				.370		.644 .708		.071 .019			15.42 16.06	A A
MOTA	1139		PHE PHE				.433 .123		.952		629			17.50	A
ATOM ATOM	1140 1141	CE2					.180		.003		571			16.80	A
ATOM	1142	CZ			146		.023	9	.126		.375			17.47	A
ATOM	1143	C	PHE	A	146		.017		.841		.783			17.00	A
MOTA	1144	0			146		.345		.308		.661 .032			19.50 17.82	A A
ATOM	1145	N CA			147 147		.950 .224		.747 .221		.377			18.67	A
MOTA MOTA	1146 1147	CB			147		.540		.604		.863			20.48	A
ATOM	1148	CG			147		.771	8	.668		.359			25.54	A
MOTA	1149	CD			147		.822		.645		.774			29.96 30.05	A A
ATOM	1150	CE			147		.835		.417		.282 .643			33.05	A
MOTA	1151 1152	NZ C			147 147		.315		.743		.338			17.25	A
ATOM ATOM	1152	Ö			147		.716		.320		.329	1.0	0	19.15	A
ATOM	1154	N	ILE	3 A	148	51	.932		.391		.428			15.47	A
MOTA	1155	CA			148	-	. 969		.846		.494			14.99	A A
MOTA	1156	CB			148		.529 .566		.424		.642 .740			15.37 14.06	Â
MOTA MOTA	1157 1158		2 ILI 1 ILI				.689		.025		.426			16.41	A
ATOM	1159		1 IL				. 223		.325	15	.550	1.0	0	18.61	A
MOTA	1160				148		2.829		.271		.682			17.07	A
MOTA	1161				148		2.721		2.702		.772			15.61 16.79	A A
ATOM	1162				149		.696 1.570		1.255		.458 .514			17.66	A
MOTA MOTA	1163 1164				. 149 . 149		5.042		1.612		.116			15.95	A
MOTA	1165				149		5.900		1.956	19	.190	1.0	0	17.31	A
ATOM	1166				149	54	.239		5.225		.763			18.34	A
MOTA	1167				149		3.854		5.949		7.842			18.33 16.95	A A
MOTA	1168				150		4.401		6.665 B.040).005).362			17.59	
MOTA	1169 1170				150 150		4.085 2.893		B.057		1.310			17.57	
MOTA MOTA	1171				150		1.679		7.314		797	1.0	00	18.52	A
MOTA	1172				150	5	0.879	1	7.851	19	789			17.12	
ATOM	1173	CE			150		9.733		7.182		9.340			18.32	_
MOTA	1174				150		1.313 0.176		6.078 5.399	_	1.345 0.901			18.89 17.65	
MOTA	1179				150 150		0.176 9.391		5.333 5.957		9.900			17.92	
MOTA MOTA	117				150		8.275		5.285	1	9.457	7 1.	00	19.69	A
ATOM	1178		TY	R A	A 150	5	5.237	7 1	8.768	2	1.02			17.16	
MOTA	1179	9 0	TY	R I	A 150	5	5.953	1	8.207	2	1.847	, 1.	υŪ	19.69	; A

1180 N LEU A 151 55.409 20.029 20.649 1.00 17.01 MOTA ATOM 1181 CA LEU A 151 56.449 20.868 21.224 1.00 15.24 MOTA 1182 CB LEU A 151 57.540 21.182 20.197 1.00 16.33 A 58.487 22.335 20.575 CG LEU A 151 1.00 16.27 ATOM 1183 MOTA 1184 CD1 LEU A 151 59.402 21.906 21.706 1.00 17.13 CD2 LEU A 151 59.315 22.755 19.359 ATOM 1185 1.00 19.34 ATOM 1186 C LEU A 151 55.825 22.174 21.666 1.00 16.08 55.221 22.881 20.860 55.952 22.497 22.945 1187 ATOM 0 LEU A 151 1.00 16.22 ATOM 1188 N THR A 152 1.00 16.84 A CA THR A 152 55.992 22.497 22.949 1.00 18.70 MOTA 1189 55.283 23.799 24.946 1.00 20.14 56.576 23.633 25.544 1.00 23.32 1190 CB THR A 152 ATOM Α MOTA 1191 OG1 THR A 152 A CG2 THR A 152 54.355 22.694 25.419 1.00 18.36 MOTA 1192 ATOM 1193 C THR A 152 56.498 24.772 23.050 1.00 20.04 57.689 24.448 1.00 20.72 THR A 152 23.034 ATOM 1194 0 56.085 25.986 22.735 1.00 20.63 MOTA 1195 N LEU A 153 A CA LEU A 153 57.043 27.014 22.389 1.00 24.69 ATOM 1196 A 57.579 26.794 MOTA 1197 CB LEU A 153 20.960 1.00 24.19 56.716 26.942 19.694 1.00 26.72 55.303 26.451 19.959 1.00 27.32 ATOM CG LEU A 153 1198 MOTA 1199 CD1 LEU A 153 MOTA 1200 CD2 LEU A 153 56.686 28.393 19.249 1.00 26.15 ATOM 1201 C LBU A 153 56.410 28.385 22.531 1.00 26.36 LEU A 153 56.410 28.385 22.531 LEU A 153 55.180 28.511 22.597 1.00 29.59 MOTA 1202 n 1203 N LEU A 154 57.262 29.401 22.620 1.00 26.29 MOTA CA LEU A 154 56.830 30.787 22.729 1.00 26.89 ATOM 1204 CA LEU A 154 56.830 30.787 22.729 1.00 26.89 CB LEU A 154 57.459 31.444 23.965 1.00 26.94 MOTA 1205 CG LEU A 154 56.966 32.833 CD1 LEU A 154 55.507 32.755 24.407 1.00 28.58 MOTA 1206 ATOM 1207 24.864 1.00 24.43 CD1 LEU A 154 55.507 32.755 24.864 1.00 24.43 CD2 LEU A 154 57.845 33.342 25.549 1.00 27.14 ATOM 1208 57.337 31.458 58.538 31.689 LEU A 154 21,456 1.00 28.94 MOTA 1209 C 1.00 30.73 21.304 ATOM 1210 0 LEU A 154 N PRO A 155 56.428 31.773 CD PRO A 155 54.975 31.534 CA PRO A 155 56.806 32.412 ATOM 1211 N 20.518 1.00 30.57 20.559 1.00 29.60 MOTA 1212 19.254 1.00 31.63 ATOM 1213 55.460 32.668 18.581 1.00 30.63 PRO A 155 MOTA 1214 CB 1215 CG PRO A 155 54.612 31.552 19.087 1.00 28.73 ATOM 57.639 33.688 19.370 1.00 33.58 MOTA 1216 C PRO A 155 57.322 34.593 58.706 33.741 PRO A 155 20.136 1.00 33.98 ATOM 1217 0 ATOM 1218 N SER A 156 18.586 1.00 35.79 1219 CA SER A 156 59.595 34.888 18.546 1.00 37.77 ATOM SER A 156 60.604 34.839 19.694 1.00 38.66 ATOM 1220 CB 59.955 34.966 SER A 156 20.949 1.00 44.00 ATOM 1221 OG 60.332 34.841 60.257 33.849 17.222 1.00 38.83 C SER A 156 ATOM 1222 ATOM 1223 0 SER A 156 16.492 1.00 38.36 61.042 35.915 ALA A 157 16.909 1.00 40.38 ATOM 1224 N 61.796 35.972 15.670 1.00 39.93 61.822 37.401 15.148 1.00 40.36 ATOM 1225 CA ALA A 157 CB ALA A 157 ATOM 1226 15.918 1.00 39.65 MOTA 1227 C ALA A 157 63.214 35.466 ALA A 157 64.058 35.504 15.021 1.00 39.72 ATOM 1228 0 63.463 34.984 ATOM 1229 N GLU A 158 17.135 1.00 39.12 64.784 34.480 65.082 34.808 17.517 1.00 40.24 ATOM CA GLU A 158 1230 18.988 1.00 44.21 ATOM 1231 CB GLU A 158 ATOM 1232 CG GLU A 158 65.426 36.268 19.287 1.00 50.31 64.204 37.174 19.356 1.00 55.36 64.353 38.351 19.765 1.00 55.75 ATOM 1233 CD GLU A 158 OE1 GLU A 158 1234 ATOM 63.095 36.712 19.002 1.00 58.12 ATOM 1235 OE2 GLU A 158 ATOM 1236 C GLU A 158 65.005 32.979 17.303 1.00 38.02 66.130 32.493 17.419 1.00 36.30 0 GLU A 158 MOTA 1237 63.950 32.234 17.002 1.00 35.79 GLU A 159 MOTA 1238 N 64.136 30.807 16.805 1.00 35.02 MOTA 1239 CA GLU A 159 **GLU A 159** 63.949 30.066 18.135 1.00 36.97 MOTA 1240 CB CG GLU A 159 62.699 30.439 18.891 1.00 41.68 MOTA 1241 62.717 29.933 20.323 1.00 44.82 MOTA 1242 CD GLU A 159 62.819 28.705 20.527 1.00 46.62 MOTA 1243 OE1 GLU A 159 1244 OE2 GLU A 159 62.631 30.767 21.248 1.00 47.25 ATOM 1245 C GLU A 159 63.277 30.162 15.735 1.00 32.21 MOTA 30.574 15.473 1.00 32.05 ATOM 1246 0 GLU A 159 62.147 29.147 15.107 1.00 29.55 ATOM 1247 N SER A 160 63.849 28.394 14.076 1.00 28.89 MOTA 1248 CA SER A 160 63.167 28.551 12.734 1.00 27.34 MOTA 1249 CB SER A 160 63.885 MOTA 1250 OG SER A 160 65.206 28.053 12.807 1.00 29.49 SER A 160 63.241 26.957 14.565 1.00 27.42 1251 C MOTA 64.092 26.628 15.392 1.00 25.45 ATOM 1252 0 SER A 160 1253 N TYR A 161 62.359 26.101 14.066 1.00 24.73 ATOM

ATOM	1254	CA	TYR	A	161	62.359	24.725	14.517	1.00 24.26	A
ATOM	1255	CB	TYR			61.172	24.480	15.451	1.00 23.50	A
ATOM	1256	CG	TYR			60.935	25.593	16.434	1.00 24.01	A
ATOM	1257		TYR			60.255	26.748	16.052	1.00 26.02	A
ATOM	1258		TYR			60.009	27.774	16.959	1.00 27.93	A
ATOM	1259		TYR			61.374	25.491	17.753	1.00 24.78	A
ATOM	1260		TYR			61.136	26.514	18.674	1.00 25.93	A
ATOM ATOM	1261 1262	CZ	TYR			60.450	27.650	18.270	1.00 27.56	A
ATOM	1263	C	TYR TYR			60.182	28.650 23.700	19.173	1.00 29.78	A
ATOM	1264	0	TYR			62.082	24.021	13.397 12.239	1.00 25.15 1.00 24.96	A
ATOM	1265	N	ASP			62.600	22.455	13.775	1.00 26.26	A A
ATOM	1266	CA	ASP			62.598	21.331	12.858	1.00 26.94	A
ATOM	1267	СВ	ASP			64.007	21.014	12.356	1.00 30.11	A
ATOM	1268	CG	ASP			64.548	22.067	11.434	1.00 32.85	A
MOTA	1269	OD1	ASP	A	162	64.075	22.138	10.277	1.00 33.31	A
MOTA	1270	OD2	ASP			65.443	22.819	11.874	1.00 33.08	A
MOTA	1271	C	asp			62.122	20.117	13.613	1.00 25.87	A
MOTA	1272	0	ASP			62.449	19.947	14.789	1.00 24.38	A
ATOM	1273	N	CYS			61.352	19.277	12.935	1.00 23.95	A
ATOM	1274	CA	CYS			60.914	18.027	13.530	1.00 24.46	A
MOTA	1275	C	CYS			61.916	17.043	12.938	1.00 22.46	A
ATOM ATOM	1276 1277	O CB	CYS			62.110 59.497	17.021	11.726 13.083	1.00 24.01 1.00 24.14	A
ATOM	1278	SG.	CYS			58.931	17.658 16.101	13.836	1.00 30.35	A A
ATOM	1279	N	LYS			62.571	16.259	13.782	1.00 22.96	A
ATOM	1280	CA	LYS			63.559	15.292	13.307	1.00 24.69	A
ATOM	1281	CB	LYS			64.867	15.450	14.089	1.00 27.54	A
ATOM	1282	CG	LYS			65.977	14.490	13.689	1.00 28.93	A
MOTA	1283	CD	LYS	A	164	67.179	14.643	14.622	1.00 32.03	A
ATOM	1284	CE	LYS	A	164	68.254	13.596	14.350	1.00 33.85	A
MOTA	1285	NZ	Lys	A	164	69.319	13.607	15.398	1.00 36.46	A
MOTA	1286	С	LYS			63.023	13.875	13.463	1.00 24.25	A
MOTA	1287	0	LYS			62.697	13.443	14.570	1.00 23.52	A
MOTA	1288	И	VAL			62.931	13.160	12.345	1.00 23.37	A
ATOM ATOM	1289 1290	CA CB	VAL VAL			62.415 61.174	11.797	12.344	1.00 24.06 1.00 23.45	A
MOTA	1291		VAL			60.657	11.682 10.248	11.408 11.382	1.00 18.80	A A
ATOM	1292		VAL			60.078	12.632	11.878	1.00 22.37	A
ATOM	1293	c	VAL			63.457	10.772	11.903	1.00 25.04	A
ATOM	1294	0	VAL			64.103	10.931	10.869	1.00 25.12	A
ATOM	1295	N	GLU	A	166	63.621	9.725	12.703	1.00 26.91	A
ATOM	1296	CA	GLU			64.556	8.648	12.383	1.00 28.84	A
MOTA	1297	CB	GLU			65.554	8.424	13.523	1.00 30.71	A
ATOM	1298	CG	GTA			66.382	9.634	13.922	1.00 36.90	A
ATOM	1299	CD	GLU			67.247	9.356	15.147	1.00 39.97	A
MOTA	1300		GLU GLU			67.466	10.286	15.954	1.00 43.02 1.00 43.24	A
ATOM ATOM	1301 1302	C	GLU			67.714 63.739	8.206 7.369	15.301 12.183	1.00 28.96	A A
ATOM	1303	ō	GLU			62.975	6.971	13.067	1.00 27.40	A
ATOM	1304	N	HIS			63.910	6.728	11.029	1.00 29.87	A
ATOM	1305	CA	HIS			63.189	5.496	10.713	1.00 30.70	A
MOTA	1306	CB	HIS			61.838	5.833	10.084	1.00 30.90	A
MOTA	1307	CG	HIS	A	167	60.932	4.655	9.933	1.00 34.01	A
ATOM	1308		HIS			60.698	3.842	8.876	1.00 33.60	A
ATOM	1309		HIS			60.159	4.172	10.967	1.00 36.69	A
ATOM	1310		HIS			59.488	3.112	10.554	1.00 34.84	A
ATOM	1311		HIS			59.798	2.890	9.290	1.00 34.90	A
atom atom	1312 1313	С 0			167 167	63.999	4.639	9.739	1.00 31.21	A
ATOM	1314	Ŋ			168	64.696 63.895	5.167 3.320	8.866 9.879	1.00 29.44	A A
ATOM	1315	CA			168	64.625	2.402	9.006	1.00 31.76	A
ATOM	1316	CB			168	64.344	0.954	9.396	1.00 30.39	A
ATOM	1317	CG			168	64.735	0.650	10.797	1.00 28.49	A
MOTA	1318		TRP			64.115	-0.297	11.666	1.00 28.31	A
MOTA	1319		TRP			64.837	-0.288	12.878	1.00 28.31	A
ATOM	1320		TRP			63.017	-1.157	11.538	1.00 26.47	A
MOTA	1321		TRP			65.778	1.184	11.491	1.00 28.32	A
ATOM	1322		TRP			65.849	0.627	12.744	1.00 28.98	A
ATOM ATOM	1323 1324		TRP TRP			64.498	-1.107	13.958	1.00 28.85	A
ATOM	1325		TRP			62.678 63.418	-1.970 -1.940	12.608 13.805	1.00 27.57 1.00 29.20	A A
ATOM	1326	C			168	64.332	2.588	7.523	1.00 23.20	Â
ATOM	1327	0			168	65.190	2.314	6.682	1.00 32.28	A

ATOM	1328	N	GLY A 169	63.126	3.049	7.202	1.00 34.81	A
MOTA	1329	CA	GLY A 169	62.760	3.263	5.810	1.00 35.23	A
ATOM	1330	C	GLY A 169	63.267 62.907	4.588 4.992	5.266	1.00 37.25	A
ATOM ATOM	1331 1332	O N	GLY A 169 LEU A 170	64.100	5.268	4.162 6.049	1.00 37.65 1.00 39.27	A A
ATOM	1333	CA	LEU A 170	64.673	6.555	5.660	1.00 41.10	A
ATOM	1334	CB	LEU A 170	64.354	7.626	6.706	1.00 38.47	A
MOTA	1335	CG	LEU A 170	62.923	8.143	6.843	1.00 38.66	A
ATOM	1336		LEU A 170		8.919	8.142	1.00 37.48	A
MOTA	1337		LEU A 170	62.572	9.017 6.425	5.653 5.556	1.00 37.65 1.00 43.62	A A
ATOM ATOM	1338 1339	C O	LEU A 170 LEU A 170	66.183 66.809	5.762	6.382	1.00 44.45	A
MOTA	1340	N	ASP A 171		7.066	4.545	1.00 46.98	A
ATOM	1341	CA	ASP A 171	68.211	7.036	4.350	1.00 48.99	A
ATOM	1342	CB	ASP A 171		7.810	3.086	1.00 51.12	A
MOTA	1343	CG	ASP A 171		7.466 7.761	1.895	1.00 53.30 1.00 54.82	A A
ATOM ATOM	1344 1345		ASP A 171 ASP A 171		6.903	1.936 0.917	1.00 54.86	A
MOTA	1346	C	ASP A 171		7.726	5.554	1.00 48.82	A
ATOM	1347	ō	ASP A 171		7.093	6.420	1.00 48.88	A
MOTA	1348	N	LYS A 172		9.044	5.585	1.00 48.96	A
MOTA	1349	CA	LYS A 172		9.877	6.659	1.00 48.79	A
ATOM	1350 1351	CB CG	LYS A 172		11.059 10.698	6.084 5.075	1.00 51.32 1.00 55.53	A A
ATOM ATOM	1351	CD	LYS A 172		11.952	4.571	1.00 57.81	A
ATOM	1353	CE	LYS A 172		11.621	3.518	1.00 59.22	A
ATOM	1354	NZ	LYS A 172		10.702	4.038	1.00 58.32	A
MOTA	1355	C	LYS A 172		10.419	7.420	1.00 46.36	A
ATOM	1356	0	LYS A 172		10.381 10.920	6.919 8.645	1.00 44.39 1.00 44.20	A A
MOTA MOTA	1357 1358	CD N	PRO A 173		10.866	9.469	1.00 44.15	A
ATOM	1359	CA	PRO A 173		11.462	9.410	1.00 42.74	A
ATOM	1360	CB	PRO A 173	67.768	12.050	10.637	1.00 42.02	A
MOTA	1361	CG	PRO A 173		11.080	10.872	1.00 44.25	A
ATOM	1362	C	PRO A 173		12.517	8.578 7.877	1.00 41.09 1.00 39.67	A A
MOTA MOTA	1363 1364	о И	PRO A 173		13.309 12.502	8.636	1.00 39.80	A
ATOM	1365	CA	LEU A 174		13.457	7.888	1.00 38.58	A
ATOM	1366	CB	LEU A 174	62.894	12.838	7.522	1.00 38.73	A
MOTA	1367	CG	LEU A 174		13.329	6.251	1.00 39.18	A
ATOM	1368	CD1			12.691	6.170	1.00 39.20 1.00 40.87	A A
MOTA MOTA	1369 1370	CD2 C	LEU A 174		14.836 14.662	6.245 8.785	1.00 37.43	A
MOTA	1371	Ö	LEU A 174		14.514	9.943	1.00 37.68	A
ATOM	1372	N	LEU A 179		15.849	8.255	1.00 35.85	A
MOTA	1373	CA	LEU A 179		17.077	9.012	1.00 34.38	A
MOTA	1374	CB	LEU A 179		17.882	9.074	1.00 33.21 1.00 34.82	A A
ATOM ATOM	1375 1376	CG	LEU A 179		17.502 17.768	10.147 11.526	1.00 34.32	Ā
MOTA	1377		LEU A 17		16.038	10.008	1.00 35.37	A
MOTA	1378	C	LEU A 175		17.898	8.337	1.00 33.09	A
MOTA	1379	0	LEU A 17		18.137	7.132	1.00 33.84	A
ATOM	1380	N	LYS A 170		18.312	9.108 8.566	1.00 30.14 1.00 30.03	A A
MOTA MOTA	1381 1382	CA CB	LYS A 170		19.119 18.416	8.772	1.00 30.60	A
ATOM	1383	CG	LYS A 17		19.049	8.010	1.00 33.60	A
ATOM	1384	CD	LYS A 17		19.054	6.508	1.00 37.73	A
MOTA	1385	CE	LYS A 17		17.642	5.960	1.00 37.37	A
MOTA	1386	NZ	LYS A 17		17.629 20.457	4.484 9.292	1.00 41.15	A A
MOTA MOTA	1387 1388	C	LYS A 17		20.524	10.501	1.00 27.68	A
MOTA	1389	N	HIS A 17		21.520	8.539	1.00 28.72	A
MOTA	1390	CA	HIS A 17		22.868	9.088	1.00 29.54	A
MOTA	1391	CB	HIS A 17		23.691	8.195	1.00 29.51	A
MOTA	1392	CG.	HIS A 17			8.663 8.114	1.00 30.53 1.00 31.99	A A
MOTA MOTA	1393 1394		R HIS A 17 L HIS A 17		26.282 25.401	9.849	1.00 32.09	A
ATOM	1395		1 HIS A 17		26.713	10.010	1.00 32.65	A
ATOM	1396		2 HIS A 17		27.271	8.971	1.00 32.04	A
MOTA	1397	С	HIS A 17		23.654	9.304	1.00 29.24	A
MOTA	1398	O N	HIS A 17		23.519 24.492	8.549 10.340	1.00 27.66 1.00 30.09	A A
MOTA MOTA	1399 1400	CA				10.540	1.00 33.43	A
MOTA	1401	CB	TRP A 17			11.632	1.00 28.07	A

ATOM	1402	CG	TRP 1	A :	178	56.	581	25.422	11.851	1.00	25.25	A
MOTA	1403		TRP A			56.4		26.518	12.761		21.68	A
MOTA	1404		TRP A			55.3 57.3		26.942 27.178	12.611 13.688		20.86	A A
ATOM ATOM	1405 1406	-	TRP 2			55.4		25.239	11.206		24.81	A
ATOM	1407		TRP A			54.		26.146	11.657		21.51	A
MOTA	1408	CZ2	TRP 2	A :	178	54.	598	27.999	13.354	1.00	21.11	A
MOTA	1409		TRP 2			56.		28.229	14.428		21.58	A
MOTA	1410		TRP A			55.		28.627	14.255		20.94	A
ATOM ATOM	1411 1412	С 0	TRP I			59. 60.		26.628 26.591	11.348 12.195		36.30 36.91	A A
ATOM	1413	N	GLU I			58.		27.761	10.975		40.65	A
ATOM	1414	CA	GLU 2			59.		29.029	11.587	1.00	45.62	A
ATOM	1415	CB	GLU 3			60.		29.622	10.899		47.42	A
ATOM	1416	CG	GLU :			60.		29.868	9.404		52.77	A
MOTA MOTA	1417 1418	CD OF 1	GLU :			61. 62.		30.624 30.179	8.806 8.987		55.17 57.20	A A
MOTA	1419		GLU :			61.		31.663	8.149		57.21	A
MOTA	1420	c	GLU :			58.		30.001	11.489		46.47	A
MOTA	1421	0	GLU :	A	179	57.	322	29.983	10.513		45.49	A
MOTA	1422	N	PRO .			57.		30.855	12.509		47.97	A
MOTA	1423	CD	PRO .			58.		31.008	13.752		48.35 49.45	A A
MOTA MOTA	1424 1425	CA CB	PRO .			56. 56.		31.810 32.372	12.460 13.880		49.39	A
MOTA	1426	CG	PRO .			58.		32.358	14.266		48.65	A
MOTA	1427	c	PRO			57.		32.891	11.401	1.00	50.21	A
MOTA	1428	0	PRO .			58.	174	33.041	10.950		49.95	A
MOTA	1429		PRO				030	33.578	11.043	-	50.90	A
ATOM	1430	CB	SER		3		953	-2.426 -3.384	7.203 6.321		59.72 60.71	B B
ATOM ATOM	1431 1432	C OG	SER SER		3 3		517 164	-3.822	9.277		57.49	В
ATOM	1433	ō	SER		3		117	-4.879	8.642		57.32	В
ATOM	1434	N	SER	В	3	70.	072	-2.418	8.486		59.35	В
MOTA	1435	CA	SER		3		586	-2.517	8.597		58.84	В
MOTA	1436	N	PRO		4		855	-3.763 -2.580	10.585 11.463		55.71 54.97	B B
MOTA MOTA	1437 1438	CD CA	PRO		4		914 438	-4.952	11.338		53.72	В
ATOM	1439	CB	PRO		4		457	-4.467	12.787		54.71	В
ATOM	1440	CG	PRO		4	67.	095	-3.021	12.660	1.00	54.93	В
ATOM	1441	С	PRO		4		069	-5.487	10.918		51.05	В
MOTA	1442	0	PRO		4		240	-4.753	10.379		50.96 47.90	B B
ATOM ATOM	1443 1444	N CA	GLU		5 5		843 581	-6.773 -7.410	11.165 10.810		45.24	В
ATOM	1445	CB	GLU		5		811	-8.893	10.489		48.23	В
MOTA	1446	CG	GLU		5	65.	603	-9.656	11.545	1.00	54.54	В
MOTA	1447	CD	GLU		5			-11.102	11.140		57.83	В
MOTA	1448		GLU		5			-11.317	10.024		59.67	B B
MOTA	1449	OE2	GLU		5 5		548	-12.020 -7.269	11.941 11.920		59.33 40.85	В
MOTA MOTA	1450 1451	0	GLU		5		876	-7.328	13.105		40.81	В
ATOM	1452	N	ASP		6		294	-7.083	11.532	1.00	36.03	В
MOTA	1453	CA	ASP		6		.223	-6.936	12.508		32.11	В
MOTA	1454	CB	ASP		6		.833	-5.460	12.616		29.96	В
MOTA	1455	CG	ASP ASP		6 6		933 280	-5.171 -4.110	13.798 13.785		27.91	B B
MOTA MOTA	1456 1457		ASP		6		884	-5.982	14.745		29.86	В
ATOM	1458	C	ASP		6		014	-7.766	12.077	1.00	29.68	В
ATOM	1459	0	ASP		6	59	.676	-7.802	10.899		29.14	В
MOTA	1460	N	PHE		7		.380	-8.438	13.032		27.77	В
ATOM	1461	CA	PHE		7		.193	-9.249 -10.704	12.765 13.161		28.11	B B
ATOM ATOM	1462 1463	CB	PHE		7 7			-11.385	12.282		31.06	В
MOTA	1464		PHE		7			-11.766	10.989		29.85	В
MOTA	1465	CD2	PHE	В	7			-11.603	12.730		32.21	В
MOTA	1466		PHE		7			-12.355	10.145		33.75	В
MOTA	1467		PHE		7			-12.190 -12.568	11.897 10.599		34.27 33.07	B B
MOTA MOTA	1468 1469	CZ	PHE		7 7		.032		13.562		26.58	В
ATOM	1470	ō	PHE				.046		14.794		25.72	В
ATOM	1471	N	VAL				.023	-8.174	12.849		25.17	В
MOTA	1472	CA	VAL				.891		13.493		23.46	В
MOTA	1473	CB	VAL				.670		12.871 13.612		21.55	В В
MOTA MOTA	1474 1475		VAL VAL				.573 .975		12.895		21.83	В
SPT OIL	13	-02	- 474	-								_

53.556 -8.255 13.467 1.00 24.08 ATOM VAL R 1476 C 8 В ATOM 1477 VAL B 53.204 -8.912 12.491 1.00 23.46 0 8 ATOM 1478 N TYR B 52.804 -8.127 14.554 1.00 23.26 ATOM TYR B 9 51.493 -8.747 14.619 1479 CA 1.00 23.18 51.510 -9.978 15.520 ATOM 1480 CB TYR B 9 1.00 23.12 В ATOM 1481 CG TYR B 9 50.231 -10.786 15.465 1.00 24.54 ATOM 1482 CD1 TYR B 9 50.158 -11.962 14.722 1.00 26.50 49.000 -12.743 14.716 MOTA 1483 CE1 TYR B 9 1.00 25.08 49.108 ~10.399 16.190 MOTA 1484 CD2 TYR B 9 1.00 22.88 ATOM 1485 CE2 TYR B 9 47.948 -11.165 16.188 1.00 23.91 ATOM 1486 CZ TYR B 9 47.902 -12.342 15.455 1.00 24.87 9 9 OH TYR B 46.780 -13.140 15.501 ATOM 1487 1.00 25.45 R MOTA 1488 С TYR B 50.509 -7.723 15.163 1.00 21.33 В 50.798 -7.028 16.133 ATOM 1489 TYR B 9 1.00 22.92 49.353 -7.622 14.521 GLN B 10 ATOM 1490 N 1.00 19.98 В 48.326 -6.687 14.952 ATOM 1491 CA GLN B 10 1.00 19.52 В ATOM 1492 CB GLN B 10 48.171 -5.523 13.962 1.00 19.13 R ATOM 1493 CG GLN B 10 49.433 -4.810 13.509 1.00 19.33 CD GLN B 10 ATOM 49.117 -3.708 12.499 1.00 17.96 1494 ATOM 1495 OE1 GLN B 10 48.336 -2.802 12.783 1.00 18.49 В 1496 NE2 GLN B 10 49.715 -3.790 .11.316 1.00 19.41 В ATOM 46.967 -7.375 15.029 ATOM 1497 C GLN B 10 1.00 19.74 46.626 -8.227 14.192 GLN B 10 В MOTA 1498 0 1.00 18.98 46.195 -6.996 16.040 1.00 19.06 ATOM 1499 N PHE B 11 R CA PHE B 11 44.842 -7.487 16.182 1.00 16.54 ATOM 1500 ATOM 1501 CB PHE B 11 44.668 -8.454 17.336 1.00 17.48 CG PHE B 11 43.237 -8.847 17.544 1.00 16.17 В ATOM 1502 ATOM 1503 CD1 PHE B 11 42.570 -9.604 16.582 1.00 17.49 CD2 PHE B 11 42.536 -8.406 18.656 1.00 14.41 ATOM 1504 В MOTA 1505 CE1 PHE B 11 41.219 -9.913 16.725 1.00 18.03 CE2 PHE B 11 41.191 -8.708 18.814 1.00 16.34 В MOTA 1506 MOTA 1507 CZ PHE B 11 40.528 -9.463 17.845 1.00 17.60 В PHE B 11 43.984 -6.271 16.450 1.00 18.14 MOTA 1508 C PHE B 11 44.241 -5.506 17.386 1.00 15.63 В MOTA 1509 0 42.961 -6.094 15.625 1.00 17.33 LYS B 12 В MOTA 1510 N MOTA 1511 CA LYS B 12 42.082 -4.958 15.770 1.00 17.63 В MOTA 1512 CB LYS B 12 42.188 -4.067 14.536 1.00 18.71 В 43.599 -3.642 14.192 1.00 15.90 MOTA 1513 CG LYS B 12 43.602 -2.909 12.871 44.946 -2.297 12.570 CD LYS B 12 1.00 17.33 В ATOM 1514 1.00 18.72 MOTA 1515 CR LYS B 12 В 1516 NZ LYS B 12 44.838 -1.450 11.340 1.00 20.93 MOTA 1.00 18.92 MOTA 1517 C LYS B 12 40.632 -5.387 15.968 LYS B 12 1.00 17.25 40.041 -6.050 15.109 В MOTA 1518 0 MOTA 1519 N GLY B 13 40.076 -5.002 17.114 1.00 17.59 В 1520 GLY B 13 38.701 -5.322 17.430 1.00 19.88 В MOTA CA 37.874 -4.113 17.064 1.00 20.12 MOTA 1521 GLY B 13 С GLY B 13 1.00 21.08 MOTA 1522 O 37.515 -3.309 17.923 В MOTA 1523 N MET B 14 37.561 -4.000 15.779 1.00 20.42 В CA MET B 14 36.817 -2.866 15.262 1.00 22.96 MOTA 1524 В MET B 14 37.334 -2.554 13.866 1.00 23.02 В ATOM 1525 CB MET B 14 38.846 -2.485 13.820 1.00 23.58 В ATOM 1526 CG ATOM 1527 SD MET B 14 39.449 -2.095 12.191 1.00 26.23 В MET B 14 39.260 -0.318 12.182 1.00 25.78 ATOM 1528 CE В 35.295 -2.997 ATOM 1529 C MET B 14 15.242 1.00 23.12 ATOM MET B 14 34.751 -4.089 15.081 1.00 24.36 1530 В 0 34.628 -1.860 ATOM 1531 N CYS B 15 15.427 1.00 24.04 В CA CYS B 15 33.173 -1.768 15.433 1.00 24.91 ATOM 1532 CYS B 15 CYS B 15 MOTA 1533 C 32.808 -0.587 14.547 1.00 25.49 33.369 0.504 14.700 1.00 23.97 MOTA В 1534 0 32.630 -1.489 16.847 1.00 26.02 ATOM 1535 CB CYS B 15 В ATOM 1536 SG CYS B 15 32.691 -2.831 18.084 1.00 33.69 В MOTA TYR B 16 31.871 -0.805 13.630 1.00 25.87 1537 N 0.244 12.724 1.00 25.59 ATOM CA TYR B 16 31.413 1538 ATOM 1539 CB TYR B 16 31.539 -0.223 11.274 1.00 24.73 ATOM 1540 CG TYR B 16 32.958 -0.575 10.879 1.00 26.05 ATOM 33.523 -1.795 11.239 1.00 22.96 1541 CD1 TYR B 16 34.843 -2.102 10.904 1.00 25.81 MOTA 1542 CB1 TYR B 16 33.748 MOTA 1543 CD2 TYR B 16 0.334 10.171 1.00 25.30 R MOTA 1544 35.066 0.041 9.835 1.00 25.12 CE2 TYR B 16 ATOM 1545 CZ TYR B 16 35.607 -1.176 10.202 1.00 26.66 MOTA 36.908 -1.463 9.868 1.00 29.22 1546 TYR B 16 OH ATOM 1547 C TYR B 16 29.960 0.575 13.045 1.00 26.48 ATOM TYR B 16 29.113 -0.315 1548 0 13.091 1.00 26.41 ATOM 1549 N PHE B 17 29.684 1.859 13.266 1.00 27.76

MOTA	1550	CA	PHE	В	17	28.346	2.338	13.613	1.00 29.09	В
ATOM	1551	CB	PHE	В	17	28.382	3.047	14.967	1.00 28.08	В
MOTA	1552	CG	PHE		17	28.885	2.194	16.091	1.00 28.21	В
ATOM	1553		PHE		17	28.056	1.253	16.693	1.00 27.20	В
MOTA	1554		PHE		17	30.188 28.519	2.340 0.470	16.558 17.752	1.00 26.60 1.00 28.13	B
MOTA MOTA	1555 1556		PHE		17 17	30.662	1.565	17.610	1.00 25.62	В
ATOM	1557	CZ	PHE		17	29.828	0.629	18.210	1.00 26.17	В
ATOM	1558	·c	PHE		17	27.772	3.318	12.592	1.00 30.71	В
MOTA	1559	ō	PHE		17	28.452	4.239	12.155	1.00 31.05	В
ATOM	1560	N	THR		18	26.506	3.125	12.237	1.00 33.51	В
MOTA	1561	CA	THR	В	18	25.831	4.005	11.291	1.00 36.95	В
MOTA	1562	CB	THR		18	25.797	3.395	9.875	1.00 37.23	В
ATOM	1563		THR		18	27.133	3.105	9.447	1.00 40.77	В
ATOM	1564	CG2	THR		18	25.171	4.369	8.891	1.00 38.43	B B
ATOM	1565	C	THR		18	24.398 23.671	4.273 3.351	11.753 12.131	1.00 38.56 1.00 38.36	В
ATOM ATOM	1566 1567	N O	THR ASN		18 19	24.007	5.544	11.726	1.00 30.30	В
ATOM	1568	CA	ASN		19	22.668	5.961	12.132	1.00 41.35	В
ATOM	1569	СВ	ASN		19	21.638	5.465	11.110	1.00 41.21	В
ATOM	1570	CG	ASN		19	20.311	6.190	11.223	1.00 42.85	В
MOTA	1571	OD1	ASN	В	19	20.271	7.378	11.548	1.00 42.24	В
ATOM	1572	ND2	asn	В	19	19.219	5.485	10.937	1.00 42.57	В
ATOM	1573	С	asn		19	22.352	5.416	13.521	1.00 42.37	В
MOTA	1574	0	ASN		19	21.540	4.503	13.673	1.00 43.36	В
ATOM	1575	N	GLY		20	22.997	5.989 5.535	14.533	1.00 42.56 1.00 43.89	B B
MOTA	1576	CA	GLY		20 20	22.790 23.293	4.110	15.894 16.031	1.00 45.10	В
ATOM ATOM	1577 1578	С 0	GLY		20	24.421	3.807	15.646	1.00 44.28	В
ATOM	1579	N	THR		21	22.458	3.232	16.575	1.00 46.37	В
ATOM	1580	CA	THR		21	22.824	1.832	16.738	1.00 47.42	В
ATOM	1581	СВ	THR		21	22.667	1.373	18.199	1.00 48.57	В
MOTA	1582	OG1	THR	В	21	21.438	1.885	18.731	1.00 49.14	В
ATOM	1583	CG2	THR	В	21	23.843	1.856	19.043	1.00 47.59	В
MOTA	1584	C	THR		21	21.958	0.947	15.846	1.00 48.74	В
MOTA	1585	0	THR		21	21.925	-0.276	16.016	1.00 48.04	В
ATOM	1586	N	GLU		22	21.253	1.570	14.902	1.00 48.57 1.00 48.90	B B
MOTA	1587	CA	GLU		22	20.405 19.741	0.822 1.745	13.979 12.957	1.00 52.60	В
ATOM	1588 1589	CB CG	GLU		22 22	18.669	2.667	13.493	1.00 58.06	В
MOTA MOTA	1590	CD	GLU		22	17.862	3.297	12.368	1.00 62.27	В
MOTA	1591		GLU		22	17.027	4.185	12.648	1.00 63.99	В
ATOM	1592		GLU		22	18.065	2.894	11.199	1.00 64.70	В
MOTA	1593	C	GLU	В	22	21.285	-0.156	13.229	1.00 46.38	В
MOTA	1594	0	GLU		22	21.029	-1.356	13.209	1.00 45.52	В
MOTA	1595	N	ARG		23	22.324	0.379	12.601	1.00 45.42	В
MOTA	1596	CA	ARG		23	23.260	-0.438	11.844	1.00 44.59 1.00 45.69	B B
MOTA	1597	CB	ARG		23	23.423 22.169	0.127	10.422 9.554	1.00 49.95	В
MOTA MOTA	1598 1599	CD	ARG		23 23	22.406	0.237	8.074	1.00 53.34	В
ATOM	1600	NE	ARG		23	22,153	1.632	7.708	1.00 55.57	В
ATOM	1601	CZ	ARG		23	20.949	2.200	7.700	1.00 57.20	В
ATOM	1602		ARG		23	19.878	1.495	8.042	1.00 58.09	В
ATOM	1603		ARG		23	20.813	3.471	7.340	1.00 56.82	В
MOTA	1604	C	ARG		23	24.606	-0.534	12.567	1.00 40.56	В
MOTA	1605	0	ARG		23	25.306	0.459	12.748	1.00 41.15	В
ATOM	1606	N	VAL		24	24.944	-1.743	12.995	1.00 38.17 1.00 34.88	B B
ATOM	1607	CA	VAL		24	26.191 25.931	-1.996 -2.314	13.708 15.200	1.00 34.41	В
MOTA MOTA	1608 1609	CB	VAL VAL		24 24	27.251	-2.526	15.918	1.00 35.28	В
ATOM	1610		VAL		24	25.146	-1.190	15.852	1.00 34.70	В
ATOM	1611	C	VAI		24	26.909	-3.194	13.100	1.00 32.34	В
ATOM	1612	0	VAI		24	26.287	-4.214	12.812	1.00 33.23	В
ATOM	1613	N	ARG	В	25	28.217	-3.076	12.898	1.00 30.18	В
ATOM	1614	CA	ARG			28.970	-4.194	12.354	1.00 26.97	В
ATOM	1615	CB	ARC			29.225	-4.022	10.852	1.00 27.67	B
ATOM	1616	CG	ARG			29.400	-5.362	10.170	1.00 29.58 1.00 31.26	B
MOTA	1617	CD	ARC			30.406 30.058	-5.363 -4.454	9.052 7.974	1.00 31.26	В
ATOM ATOM	1618 1619	NE CZ		3 B 3 B		30.415	-4.631	6.705	1.00 32.27	В
ATOM	1620		L ARC			31.124	-5.695	6.346	1.00 31.13	В
ATOM	1621		2 ARC			30.087	-3.726	5.799	1.00 30.62	В
ATOM	1622	C		3 B		30.305	-4.402	13.065	1.00 24.10	В
MOTA	1623	0	AR	3 B	25	31.095	-3.477	13.225	1.00 22.56	В

ATOM	1624	N	LEU !	В	26	30.551	-5.630	13.495	1.00 22.65	В
ATOM	1625	CA	LEU I	В	26	31.801	-5.942	14.163	1.00 22.38	В
MOTA	1626	CB	LEU I		26	31.558	-6.888	15.345	1.00 20.25	В
ATOM	1627	CG	LEU :		26	32.795	-7.389	16.100	1.00 19.86	В
MOTA	1628		LEU :		26	32.452	-7.613	17.568	1.00 22.49	B
MOTA MOTA	1629 1630	CD2	LEU :		26 26	33.304 32.726	-8.665 -6.591	15.464 13.150	1.00 18.43 1.00 21.50	В
ATOM	1631	ō	LEU :		26	32.720	-7.402	12.342	1.00 22.83	В
ATOM	1632	N	VAL		27	33.998	-6.208	13.177	1.00 21.29	В
ATOM	1633	CA	VAL		27	34.984	-6.780	12.270	1.00 20.66	В
ATOM	1634	CB	VAL :		27	35.178	-5.911	11.004	1.00 20.59	В
MOTA	1635	CG1	VAL :	В	27	36.169	-6.576	10.069	1.00 19.45	В
MOTA	1636	CG2	VAL :	В	27	33.849	-5.696	10.297	1.00 22.37	В
ATOM	1637	C	VAL :		27	36.330	-6.885	12.988	1.00 22.39	В
ATOM	1638	0	VAL		27	37.046	-5.889	13.135	1.00 22.63	В
MOTA	1639	N	SER		28	36.673	-8.083	13.450	1.00 21.32 1.00 21.51	B B
ATOM ATOM	1640 1641	CA CB	SER		28 28	37.947 37.831	-8.259 -9.284	14.130 15.275	1.00 21.31	В
ATOM	1642	OG	SER		28		-10.581	14.819	1.00 24.33	В
ATOM	1643	C	SER		28	38.954	-8.693	13.074	1.00 21.25	В
ATOM	1644	ō	SER		28	38.661	-9.537	12.229	1.00 19.44	В
ATOM	1645	N	ARG	В	29	40.137	-8.089	13.106	1.00 20.61	В
ATOM	1646	CA	ARG	В	29	41.158	-8.402	12.115	1.00 19.66	В
ATOM	1647	CB	ARG	В	29	41.418	-7.169	11.230	1.00 19.91	В
MOTA	1648	CG	ARG		29	40.178	-6.407	10.754	1.00 16.79	В
ATOM	1649	CD	ARG		29	40.608	-5.121	10.031	1.00 18.10	В
ATOM	1650	NE	ARG		29	39.487	-4.318	9.553	1.00 19.38	B B
MOTA	1651	CZ	ARG ARG		29 29	38.738 38.983	-4.619 -5.714	8.497 7.789	1.00 20.62 1.00 19.50	В
MOTA MOTA	1652 1653		ARG		29	37.736	-3.714	8.149	1.00 21.90	В
ATOM	1654	C	ARG		29	42.482	-8.833	12.738	1.00 18.57	В
MOTA	1655	ō	ARG		29	43.024	-8.121	13.584	1.00 19.40	В
MOTA	1656	N	SER		30	42.991	-9.995	12.326	1.00 18.99	В
ATOM	1657	CA	SER	В	30	44.284	-10.501	12.797	1.00 21.66	В
ATOM	1658	CB	SER	В	30	44.241	-12.015	13.023	1.00 22.77	В
MOTA	1659	OG	SER	В	30		-12.352	14.106	1.00 26.81	В
ATOM	1660	C	SER		30		-10.163	11.673	1.00 23.37	В
MOTA	1661	0	SER		30		-10.553	10.522	1.00 21.31	В
MOTA	1662	N	ILE		31	46.338	-9.450	12.009	1.00 24.76 1.00 24.33	B B
ATOM	1663	CA CB	ILE		31 31	47.298 47.341	-8.998 -7.440	10.999 10.958	1.00 25.20	В
MOTA MOTA	1664 1665		ILE		31	47.982	-6.964	9.672	1.00 23.24	В
ATOM	1666		ILE		31	45.934	-6.857	11.106	1.00 26.96	В
ATOM	1667		ILE		31	45.032	-7.136	9.947	1.00 31.25	В
ATOM	1668	C	ILE		31	48.741	-9.460	11.187	1.00 23.98	В
ATOM	1669	0	IFE	В	31	49.298	-9.318	12.272	1.00 22.29	В
ATOM	1670	N	TYR		32	49.345	-9.993	10.123	1.00 25.50	В
ATOM	1671	CA	TYR		32		-10.405	10.162	1.00 26.21	В
ATOM	1672	CB	TYR		32		-11.764	9.492	1.00 28.46 1.00 31.10	B B
ATOM	1673	CG	TYR		32 32		-12.224 -12.412	9.544 10.765	1.00 32.47	В
ATOM ATOM	1674 1675		TYR		32		-12.780	10.703	1.00 34.69	В
ATOM	1676		TYR		32		-12.424	8.375	1.00 33.60	В
ATOM	1677		TYR		32		-12.795	8.422	1.00 34.50	В
ATOM	1678	CZ	TYR		32	55.103	-12.965	9.654	1.00 35.65	В
MOTA	1679	OH	TYR	В	32	56.438	-13.281	9.717	1.00 37.73	В
MOTA	1680	C	TYR	В	32	51.478	-9.307	9.384	1.00 25.67	В
MOTA	1681	0	TYR		32	51.273	-9.140	8.174	1.00 24.75	В
MOTA	1682	N	ASN		33	52.319	-8.559	10.094	1.00 25.63	В
ATOM	1683	CA	ASN		33	53.036 53.955	-7.416	9.526 8.379	1.00 24.95 1.00 23.75	B B
MOTA MOTA	1684 1685	CB	asn asn		33 33	55.171	-7.848 -8.615	8.878	1.00 24.11	В
ATOM	1686		LASN		33	55.803	-8.223	9.861	1.00 25.42	В
ATOM	1687		ASN		33	55.506	-9.708	8.204	1.00 25.18	В
ATOM	1688	C	ASN		33	51.990		9.070	1.00 25.11	В
ATOM	1689	o	ASN		33	51.491	-5.618	9.893	1.00 26.06	В
MOTA	1690	'n	ARG		34	51.652		7.786	1.00 25.75	В
MOTA	1691	CA	ARG		34	50.631		7.296	1.00 27.64	В
ATOM	1692	CB	ARG		34	51.244		6.408	1.00 27.74	В
ATOM	1693	CG	ARG		34	51.972 51.664		7.158 6.541	1.00 29.94 1.00 32.95	B B
ATOM ATOM	1694	NE	ARG ARG		34 34	51.897		5.101	1.00 32.33	В
ATOM	1695 1696	CZ	ARG		34	51.392		4.267	1.00 37.51	В
MOTA	1697		L ARG		34	50.622		4.729	1.00 39.45	В

ATOM 1698 NH2 ARG B 34 51.642 -1.058 2.967 1.00 36.90 ATOM 1699 C ARG B 34 49.587 -6.218 6.498 1.00 26.48 ARG B 34 48.740 -5,639 MOTA 1700 0 5.825 1.00 27.17 ATOM 1701 N GLU B 35 49.647 -7.534 6.602 1.00 25.66 ATOM 1702 CA GLUB 35 48.746 - -8.394 5.867 1.00 26.99 49.570 -9.483 GLU B 35 MOTA 1703 CB 5.175 1.00 31.53 В ATOM 1704 CG GLU B 35 48.814 -10.396 4.235 1.00 36.29 CD GLUB 35 49.695 -11.530 MOTA 1705 3.731 1.00 40.61 ATOM 1706 OB1 GLU B 35 50.825 -11.240 3.276 1.00 45.20 R OE2 GLU B 35 49.266 -12.705 ATOM 1707 3.791 1.00 41.13 В ATOM 1708 C GLU B 35 47.699 -9.031 6.764 1.00 25.09 В ATOM 1709 0 GLU B 35 48.028 -9.807 7.663 1.00 23.31 46.439 -8.689 GLU B 36 6.522 1.00 24.53 MOTA 1710 N 1711 CA GLU B 36 45.332 -9.263 MOTA 7.275 1.00 25.73 R 44.023 -8.519 MOTA 1712 CB GLU B 36 6.958 1.00 26.62 В 42.783 -9.095 MOTA 1713 CG GLU B 36 7.636 1.00 28.26 CD GLUB 36 41.545 -8.232 1714 MOTA 7.442 1.00 31.08 В 41.420 -7.590 OR1 GLU B 36 1.00 32.56 ATOM 1715 6.377 В MOTA 1716 OE2 GLU B 36 40.685 -8.206 8.349 1.00 32.83 ATOM 1717 C GLU B 36 45.238 -10.717 6.822 1.00 24.67 GLU B 36 45.141 -10.992 5.626 1.00 23.91 MOTA 1718 0 В ILE B 37 MOTA 1719 N 45.282 -11.647 7.771 1.00 26.11 В ATOM 1720 CA ILE B 37 45.219 -13.067 7,433 1.00 27.80 В MOTA 1721 CB ILE B 37 46.444 -13.822 8.013 1.00 27.27 47.728 -13.174 ATOM 1722 CG2 ILE B 37 7.516 1.00 27.41 B 46.440 -13.767 ATOM 1723 CG1 ILE B 37 9.537 1.00 29.35 В 1724 CD1 ILE B 37 47.596 -14.509 10.175 1.00 30.27 В MOTA ATOM 1725 C ILE B 37 43.922 -13.750 7.879 1.00 27.86 ILE B 37 43.445 -14.674 7.221 1.00 28.29 ATOM 1726 O VAL B 38 43.348 -13.296 8.989 1.00 28.78 1727 N ATOM В CA VAL B 38 42.097 -13.870 MOTA 1728 9.487 1.00 29.29 В ATOM 1729 CB VAL B 38 42.294 -14.751 10.741 1.00 30.18 ATOM 1730 CG1 VAL B 38 40.983 -15.452 11.071 1.00 33.17 43.399 -15.764 10.520 1731 CG2 VAL B 38 1.00 31.09 ATOM MOTA 1732 C VAL B 38 41.161 -12.745 9.882 1.00 28.75 В VAL B 38 41.585 -11.758 10.480 1.00 29.70 MOTA 1733 0 В 39.881 -12.911 9.581 1.00 27.05 ATOM 1734 N ARG B 39 38.895 -11.890 38.627 -11.064 1735 CA ARG B 39 9.892 1.00 25.46 ATOM В MOTA 1736 CB ARG B 39 8.632 1.00 27.23 В 37.544 -10.011 8.765 1.00 30.84 MOTA 1737 CG ARG B 39 1738 CD ARG B 39 37.111 -9.476 . 7.398 1.00 29.34 ATOM 38.218 -8.861 6.673 1.00 30.83 ATOM 1739 NE ARG B 39 В 1740 CZ ARG B 39 38.116 -8.328 5.459 1.00 31.23 ATOM ATOM 1741 NH1 ARG B 39 36.951 -8.333 4.823 1.00 31.08 39.178 -7.779 1.00 30.81 ATOM 1742 NH2 ARG B 39 4.883 1743 C ARG B 39 37.573 -12.476 10.381 1.00 25.41 ATOM Ŕ ATOM 1744 ARG B 39 37.192 -13.587 9.996 1.00 25.06 0 36.890 -11.742 ATOM 1745 N PHE B 40 11,252 1.00 23.72 1746 CA PHE B 40 35.569 -12.164 11.696 1.00 24.04 В ATOM 35.498 -12.554 13.171 1.00 22.69 CB PHE B 40 ATOM 1747 В 34.133 -13.036 MOTA 1748 CG PHE B 40 13.573 1.00 20.75 В 33.777 -14.370 1.00 21.07 MOTA 1749 CD1 PHE B 40 13.413 CD2 PHE B 40 33.162 -12.135 14.003 1.00 21.00 ATOM 1750 32.475 -14.800 13.670 1.00 20.86 CE1 PHE B 40 В ATOM 1751 31.858 -12.553 ATOM 1752 CE2 PHE B 40 14.261 1.00 19.95 В CZ PHE B 40 MOTA 1753 31.517 -13.890 14.092 1.00 19.78 C PHE B 40 34.662 -10.969 11.474 1.00 24.27 ATOM 1754 12.183 1.00 22.94 PHE B 40 34.755 -9.970 В ATOM 1755 10.471 1.00 24.75 MOTA 1756 N ASP B 41 33.800 -11.088 R CA ASP B 41 32.857 -10.040 10.101 1.00 24.98 В ATOM 1757 8.578 1.00 25.64 CB ASP B 41 32.863 -9.881 MOTA 1758 CG ASP B 41 32.162 -8.626 8.116 1.00 27.70 В ATOM 1759 8.749 1.00 26.21 MOTA 1760 OD1 ASP B 41 31.163 -8.227 OD2 ASP B 41 32.607 -8.045 7.102 1.00 30.42 MOTA 1761 ASP B 41 31.477 -10.497 1.00 24.50 1762 10.560 MOTA C ASP B 41 31.011 -11.558 10.151 1.00 24.95 MOTA 1763 0 11.404 1.00 24.16 SER B 42 30.822 -9.710 MOTA 1764 N 11.882 1.00 26.13 1765 CA SER B 42 29.501 -10.096 MOTA 29.013 -9.133 12.972 1.00 24.53 ATOM 1766 CB SER B 42 SER B 42 28.932 -7.806 12.497 1.00 23.39 ATOM 1767 OG 10.729 1.00 27.68 SER B 42 28.497 -10.149 ATOM 1768 С 10.818 1.00 27.31 1769 0 SER B 42 27.474 -10.833 MOTA ASP B 43 28.789 -9.419 9.654 1.00 28.17 ATOM 1770 N 1771 CA ASP B 43 27.924 -9.413 MOTA 8.477 1.00 29.40

ATOM	1772	СВ	ASP	В	43	28.332 -8.298 7.508 1.00 29.57	В
ATOM	1773	CG	ASP	В	43	27.587 -7.006 7.766 1.00 32.71	В
MOTA	1774		ASP		43	26.999 -6.868 8.862 1.00 33.94	В
MOTA	1775		ASP		43	27.593 -6.120 6.881 1.00 33.98	В
ATOM	1776	C	ASP		43	28.036 -10.762	B B
ATOM ATOM	1777 1778	O N	ASP VAL		44	29.123 -11.471 8.068 1.00 27.98	В
ATOM	1779	CA	VAL		44	29.365 -12.780 7.486 1.00 27.16	В
ATOM	1780	СВ	VAL		44	30.846 -12.939 7.075 1.00 27.32	В
ATOM	1781		VAL		44	31.083 -14.323 6.488 1.00 24.09	В
ATOM	1782		VAL		44	31.218 -11.857 6.073 1.00 24.66	В
MOTA	1783	C	VAL	В	44	28.990 -13.867 8.490 1.00 28.43	В
MOTA	1784	0	VAL	В	44	28.558 -14.948 8.108 1.00 29.45	В
ATOM	1785	N	GLY		45	29.177 -13.590 9.774 1.00 28.05	В
ATOM	1786	CA	GLY		45	28.794 -14.561 10.780 1.00 28.67	В
MOTA	1787	C	GLY		45	29.758 -15.679 11.125 1.00 28.25	В
MOTA	1788	0	GLY		45	29.458 -16.486 12.002 1.00 29.67	B B
ATOM	1789	N	GLU		46 46	30.895 -15.755 10.443 1.00 27.03 31.873 -16.787 10.757 1.00 29.26	В
MOTA MOTA	1790 1791	CA CB	GLU		46	31.571 -18.087 10.000 1.00 32.16	В
ATOM	1792	CG	GLU		46	32.039 -18.121 8.554 1.00 37.36	В
ATOM	1793	CD	GLU		46	31.752 -19.458 7.885 1.00 41.59	В
ATOM	1794		eru		46	32.163 -20.505 8.433 1.00 43.30	В
ATOM	1795	OE2	GLU	В	46	31.116 -19.463 6.810 1.00 43.54	В
MOTA	1796	C	GLU	В	46	33.272 -16.295 10.413 1.00 29.29	В
ATOM	1797	0	GLU	В	46	33.432 -15.288 9.722 1.00 30.45	В
ATOM	1798	N	PHE		47	34.281 -17.005 10.904 1.00 28.00	В
ATOM	1799	CA	PHE		47	35.670 -16.650 10.651 1.00 28.10	В
ATOM	1800	CB	PHE		47	36.594 -17.445 11.566 1.00 28.74 36.487 -17.067 13.016 1.00 30.23	B
ATOM	1801 1802	CG	PHE		47 47	36.487 -17.067 13.016 1.00 30.23 37.248 -16.023 13.535 1.00 28.96	В
ATOM ATOM	1803		PHE		47	35.636 -17.768 13.870 1.00 30.80	В
ATOM	1804		PHE		47	37.166 -15.683 14.888 1.00 31.59	В
ATOM	1805		PHE		47	35.544 -17.435 15.229 1.00 31.97	В
ATOM	1806	CZ	PHE		47	36.311 -16.392 15.737 1.00 30.36	В
ATOM	1807	C	PHE	В	47	36.034 -16.948 9.211 1.00 28.71	В
MOTA	1808	0	PHE	В	47	35.576 -17.937 8.640 1.00 28.03	В
MOTA	1809	N	ARG		48	36.872 -16.091 8.637 1.00 27.96	В
MOTA	1810	CA	ARG		48	37.327 -16.242 7.261 1.00 26.41	В
ATOM	1811	CB	ARG		48	36.513 -15.341 6.326 1.00 26.57 35.068 -15.755 6.108 1.00 26.19	B B
MOTA	1812	CG	ARG ARG		48 48	35.068 -15.755 6.108 1.00 26.19 34.971 -17.079 5.352 1.00 24.98	В
ATOM ATOM	1813 1814	NE CD	ARG		48	33.579 -17.465 5.146 1.00 26.01	В
ATOM	1815	CZ	ARG		48	32.755 -16.867 4.294 1.00 26.84	В
ATOM	1816		ARG		48	33.181 -15.857 3.554 1.00 26.92	В
ATOM	1817		ARG		48	31.492 -17.260 4.204 1.00 30.22	В
ATOM	1818	Ċ	ARG		48	38.799 -15.861 7.140 1.00 26.95	В
MOTA	1819	0	ARG	В	48	39.255 -14.878 7.737 1.00 24.36	В
MOTA	1820	N	ALA		49	39.542 -16.647 6.373 1.00 24.93	В
ATOM	1821	CA	ALA		49	40.943 -16.349 6.143 1.00 26.58	В
MOTA	1822	СВ	ALA		49	41.709 -17.619 5.792 1.00 27.05	B B
MOTA	1823	C	ALA		49	40.927 -15.397 4.956 1.00 26.47 40.210 -15.635 3.983 1.00 26.12	В
MOTA	1824	0	ALA VAL		49 50	40.210 -15.635 3.983 1.00 26.12 41.674 -14.302 5.044 1.00 27.06	В
MOTA MOTA	1825 1826	N CA	VAL		50	41.720 -13.357 3.936 1.00 26.50	В
MOTA	1827	CB	VAL		50	41.790 -11.876 4.439 1.00 27.14	В
ATOM	1828		. VAL		50	42.327 -11.827 5.846 1.00 29.89	В
ATOM	1829		VAL		50	42.628 -11.020 3.501 1.00 27.33	В
ATOM	1830	C	VAL	В	50	42.891 -13.742 3.037 1.00 26.58	В
MOTA	1831	0	VAL		50	42.914 -13.390 1.860 1.00 27.84	В
MOTA	1832	N	THR		51	43.842 -14.489 3.598 1.00 26.61	В
MOTA	1833	CA	THR		51	44.992 -15.011 2.846 1.00 28.59	В
MOTA	1834	СВ	THR		51	46.295 -14.193 3.056 1.00 28.25 46.828 -14.464 4.356 1.00 28.56	В
ATOM	1835		THR		51 51	46.828 -14.464 4.356 1.00 28.56 46.033 -12.699 2.899 1.00 27.40	B
ATOM	1836	CG2	THR		51 51	45.256 -16.435 3.344 1.00 29.29	В
MOTA MOTA	1837 1838	0	THR		51	44.787 -16.818 4.418 1.00 30.16	В
ATOM	1839	и	LEU		52	46.005 -17.217 2.575 1.00 30.64	В
MOTA	1840	CA	LEU		52	46.309 -18.596 2.959 1.00 31.32	В
ATOM	1841	СВ	LEU		52	47.277 -19.237 1.963 1.00 32.19	В
ATOM	1842	CG	LEU		52	46.706 -19.724 0.624 1.00 36.90	В
MOTA	1843		LEU		52	47.836 -20.306 -0.216 1.00 35.68	В
ATOM	1844		LEU		52 52	45.620 -20.775	B
ATOM	1845	C	LEU	В	52	46.892 -18.724 4.359 1.00 31.57	5

ATOM	1846	0	LEU B	52	46.570 -19.656	5.097	1.00 31.50	В
ATOM	1847	N	LEU B	53	47.753 -17.786	4.723	1.00 31.09	В
ATOM	1848	CA	LEU B	53	48.388 -17.815	6.029	1.00 30.93	В
ATOM ATOM	1849 1850	CB	TEA B	53 53	49.160 -16.511 50.338 -16.532	6.246 7.221	1.00 31.99 1.00 35.20	B B
ATOM	1851		LEU B	53	51.364 -17.559	6.763	1.00 35.92	В
MOTA	1852		LEU B	53	50.975 -15.148	7.284	1.00 34.96	В
ATOM	1853	C	LEU B	53	47.377 -18.017	7.160	1.00 29.90	В
MOTA	1854	0	TEO B	53	47.663 -18.709	8.138	1.00 30.68	В
ATOM	1855	N	GLY B	54	46.192 -17.430	7.015 8.057	1.00 28.63 1.00 29.75	B B
MOTA MOTA	1856 1857	CA C	GLY B	54 54	45.181 -17.537 44.140 -18.635	7.901	1.00 30.44	В
ATOM	1858	ō	GLY B	54	43.146 -18.664	8.630	1.00 28.02	В
ATOM	1859	N	LEU B	55	44.364 -19.547	6.964	1.00 30.54	В
MOTA	1860	CA	TEA B	55	43.417 -20.630	6.732	1.00 32.59	В
ATOM	1861	CB	LEU B	55	43.765 -21.344	5.422	1.00 35.94 1.00 38.88	В
ATOM ATOM	1862 1863	CD1	LEU B	55 55	42.776 -22.383 41.355 -21.831	4.889 4.927	1.00 38.23	B B
ATOM	1864		LEU B	55	43.173 -22.766	3.467	1.00 39.03	В
ATOM	1865	C	LEU B	55	43.330 -21.631	7.892	1.00 32.20	В
MOTA	1866	0	TER B	55	42.235 -22.026	8.291	1.00 33.32	В
ATOM	1867	N	PRO B	56	44.478 -22.058	8.447	1.00 31.03	B
ATOM	1868	CD	PRO B	56 56	45.862 -21.802 44.451 -23.013	8.009 9.561	1.00 30.17 1.00 30.23	В
MOTA MOTA	1869 1870	CA CB	PRO B	56	45.925 -23.148	9.931	1.00 30.27	В
MOTA	1871	CG	PRO B	56	46.609 -22.967	8.610	1.00 28.92	В
MOTA	1872	C	PRO B	56	43.613 -22.525	10.740	1.00 31.42	В
MOTA	1873	0	PRO B	56	42.730 -23.237	11.222	1.00 33.17	В
MOTA	1874	N	ALA B	57	43.893 -21.305	11.196	1.00 30.04 1.00 28.60	B B
ATOM ATOM	1875 1876	CA CB	ALA B ALA B	57 57	43.181 -20.719 43.818 -19.389	12.322 12.697	1.00 26.80	В
ATOM	1877	c	ALA B	57	41.695 -20.528	12.021	1.00 29.08	В
ATOM	1878	o	ALA B	57	40.847 -20.737	12.887	1.00 28.22	В
ATOM	1879	N	ALA B	58	41.385 -20.135	10.791	1.00 28.84	В
MOTA	1880	CA	ALA B	58	40.002 -19.922	10.386	1.00 31.06	B B
MOTA	1881	СВ	ALA B	58 58	39.955 -19.426 39.169 -21.199	8.947 10.529	1.00 29.79 1.00 32.38	В
ATOM ATOM	1882 1883	C	ALA B	58	38.113 -21.197	11.170	1.00 31.57.	В
ATOM	1884	N	GLU B	59	39.647 -22.285	9.929	1.00 33.50	В
ATOM	1885	CA	GLU B	59	38.949 -23.565	9.993	1.00 33.91	В
MOTA	1886	CB	GLT B	59	39.706 -24.622	9.195	1.00 35.67	В
ATOM	1887	CG	GLU B	59	39.619 -24.457	7.696	1.00 39.73 1.00 43.58	B B
ATOM ATOM	1888 1889	CD	GLUB GLUB	59 59	40.327 -25.583 41.561 -25.715	6.957 7.119	1.00 44.52	В
ATOM	1890	OE2		59	39.648 -26.337	6.222	1.00 44.30	В
ATOM	1891	C	GLU B	59	38.771 -24.063	11.425	1.00 33.56	В
MOTA	1892	0	GLU B	59	37.708 -24.570	11.790	1.00 34.40	В
MOTA	1893	N	TYR B	60	39.815 -23.923	12.233 13.611	1.00 31.99 1.00 31.01	B B
MOTA MOTA	1894 1895	CA CB	TYR B	60 60	39.754 -24.369 41.112 -24.202	14.292	1.00 31.01	В
ATOM	1896	CG	TYR B		41.051 -24.548	15.750	1.00 30.99	В
ATOM	1897		TYR B		40.919 -25.871	16.162	1.00 32.55	В
ATOM	1898		TYR B		40.770 -26.192	17.508	1.00 35.39	В
MOTA	1899		TYR B		41.039 -23.550		1.00 32.67 1.00 35.14	B B
MOTA MOTA	1900 1901	CEZ	TYR B		40.890 -23.853 40.756 - 25.177		1.00 36.91	В
ATOM	1902	OH	TYR B		40.606 -25.483		1.00 40.06	В
ATOM	1903	C	TYR B		38.695 -23.631		1.00 31.72	В
MOTA	1904	0	TYR B		37.840 -24.258		1.00 31.72	В
MOTA	1905	N	TRP B		38.752 -22.303		1.00 30.37 1.00 31.57	B B
ATOM ATOM	1906 1907	CA CB	TRP B		37.790 -21.525 38.129 -20.024		1.00 32.14	В
ATOM	1908	CG	TRP B		39.430 -19.666		1.00 33.73	В
MOTA	1909		TRP B		40.359 -18.648		1.00 35.16	В
ATOM	1910		TRP B		41.418 -18.662		1.00 35.99	В
MOTA	1911		TRPB		40.397 -17.719		1.00 38.30	B
MOTA MOTA	1912 1913		1 TRP B 1 TRP B		39.949 -20.236 41.142 -19.642			В
ATOM	1913		2 TRP B		42.512 -17.782			В
MOTA	1915		3 TRP E		41.487 -16.836	14.293	1.00 39.26	В
MOTA	1916		2 TRP E		42.527 -16.879			В
MOTA	1917		TRP E		36.349 -21.758 35.436 -21.758			B B
MOTA MOTA	1918 1919	о И	ASN E		36.137 ~21.955			В
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ATOM	1920	CA	ASN	В	62	34.781 -22.191 12.950 1.00 32.57	В
ATOM	1921	CB	ASN	В	62	34.701 -22.021 11.434 1.00 30.37	В
ATOM	1922	CG	asn		62	34.575 -20.574 11.025 1.00 29.69	В
MOTA	1923		ASN		62	33.889 -19.794 11.680 1.00 29.42	В
ATOM	1924		ASN		62	35.222 -20.209	B B
MOTA MOTA	1925 1926	C	asn asn		62 62	33.028 -23.789 13.292 1.00 34.70	В
ATOM	1927	N	SER		63	35.128 -24.469 13.725 1.00 32.43	В
ATOM	1928	CA	SER		63	34.705 -25.797 14.140 1.00 32.38	В
MOTA	1929	CB	SER		63	35.818 -26.819 13.879 1.00 32.20	В
MOTA	1930	OG	SER	В	63	36.905 -26.626 14.760 1.00 33.33	В
MOTA	1931	C	SER		63	34.348 -25.768 15.630 1.00 32.14	В
MOTA	1932	0	SER		63	33.677 -26.667 16.138 1.00 32.86	В
MOTA	1933	N	GLN		64 64	34.794 -24.724 16.325 1.00 31.10 34.513 -24.569 17.752 1.00 30.99	B B
ATOM ATOM	1934 1935	CA CB	GLN GLN		64	35.661 -23.837 18.446 1.00 32.54	В
MOTA	1936	CG	GLN		64	36.988 -24.557 18.383 1.00 34.49	В
ATOM	1937	cm	GLN		64	36.870 -25.998 18.810 1.00 38.20	В
ATOM	1938		GLN		64	36.629 -26.884 17.984 1.00 40.82	В
ATOM	1939	NE2	GLN	В	64	37.022 -26.245 20.108 1.00 38.34	В
MOTA	1940	C	GLN		64	33.226 -23.775 17.944 1.00 29.88	В
MOTA	1941	0	GLN		64	33.252 -22.549	B
ATOM	1942	N	LYS		65 65	32.101 -24.476 17.979 1.00 28.74 30.815 -23.812 18.123 1.00 29.18	В
ATOM ATOM	1943 1944	CA CB	LYS		65	29.688 -24.851 18.132 1.00 30.63	В
ATOM	1945	CG	LYS		65	29.575 -25.612 16.812 1.00 32.20	В
ATOM	1946	CD	LYS		65	29.371 -24.654 15.629 1.00 34.44	В
MOTA	1947	CE	LYS		65	29.688 -25.327 14.284 1.00 37.24	В
MOTA	1948	NZ	LYS		65	29.430 -24.427 13.109 1.00 37.89	В
MOTA	1949	С	LYS		65	30.745 -22.919 19.352 1.00 28.19	В
ATOM	1950	0	LYS		65	30.075 -21.891 19.333 1.00 28.16	В
ATOM	1951	N	ASP ASP		66 66	31.440 -23.304 20.417 1.00 27.58 31.460 -22.504 21.636 1.00 27.41	B B
MOTA MOTA	1952 1953	CA. CB	ASP		66	32.283 -23.208 22.727 1.00 28.45	В
ATOM	1954	CG	ASP		66	33.559 -23.847 22.184 1.00 32.24	В
ATOM	1955		ASP		66	33.478 -24.591 21.183 1.00 33.17	В
ATOM	1956	OD2	ASP	В	66	34.642 -23.623 22.765 1.00 33.25	В
MOTA	1957	C	ASP		66	32.050 -21.131 21.316 1.00 26.63	В
MOTA	1958	0	ASP		66	31.468 -20.102 21.662 1.00 24.32	В
MOTA	1959	N	ILE		67	33.198 -21.116	B B
ATOM ATOM	1960 1961	CA CB	ILE		67 67	33.840 -19.855 20.273 1.00 26.42 35.206 -20.088 19.613 1.00 28.29	В
ATOM	1962		ILE		67	35.859 -18.753 19.290 1.00 28.54	В
ATOM	1963		ILE		67	36.094 -20.925 20.535 1.00 28.25	В
ATOM	1964	CD1	ILB	В	67	36.319 -20.321 21.906 1.00 32.66	В
MOTA	1965	C	ILE	В	67	32.968 -19.061 19.300 1.00 26.36	В
MOTA	1966	0	ILE		67	32.747 -17.869 19.491 1.00 25.33	В
ATOM	1967	N	PEA		68	32.472 -19.730 18.261 1.00 26.11 31.617 -19.086 17.267 1.00 26.66	B B
ATOM ATOM	1968 1969	CA CB	LEU		68 68	31.617 -19.086 17.267 1.00 26.66 31.132 -20.102 16.235 1.00 27.61	В
MOTA	1970	CG	LEU		68	31.807 -20.171 14.872 1.00 30.12	В
MOTA	1971		LEU		68	31.081 -21.216 14.031 1.00 33.09	В
ATOM	1972	CD2	LEU	В	68	31.766 -18.812 14.190 1.00 30.01	В
MOTA	1973	C	ΓEΩ		68	30.394 -18.415 17.878 1.00 26.81	В
MOTA	1974	0	LEU		68	30.067 -17.280 17.541 1.00 26.19	В
ATOM	1975	N	GLU		69 60	29.706 -19.135	B B
MOTA MOTA	1976 1977	CA CB	GLU GLU		69 69	27.945 -19.654 20.382 1.00 35.75	В
MOTA	1978	CG	GLU		69	27.304 -20.862 19.695 1.00 43.71	В
ATOM	1979	CD	GLU		69	26.883 -21.954 20.673 1.00 47.92	В
ATOM	1980	OE1	. GLU	В	69	27.756 -22.454 21.418 1.00 49.27	В
MOTA	1981		GLU		69	25.683 -22.316 20.694 1.00 50.44	В
MOTA	1982	C	GLU		69	28.773 -17.295 20.130 1.00 29.82	В
MOTA	1983	0	GLU		69 70	27.986 -16.356 20.027 1.00 27.91 29.886 -17.226 20.855 1.00 29.32	B B
MOTA	1984 1985	N CA	ARG ARG		70 70	29.886 -17.226	В
MOTA MOTA	1985	CB	ARG		70	31.347 -16.315 22.606 1.00 28.94	В
ATOM	1987	CG	ARG		70	30.982 -17.344 23.673 1.00 30.55	В
MOTA	1988	CD	ARG		70	32.251 -17.810 24.371 1.00 32.35	В
MOTA	1989	NE	ARG		70	32.040 -19.037 25.117 1.00 34.83	В
MOTA	1990	CZ	ARG		70	32.946 -19.997 25.232 1.00 34.98	В
MOTA	1991		L ARG		70 70	34.131 -19.875 24.647 1.00 35.03 32.662 -21.083 25.930 1.00 39.48	B B
MOTA MOTA	1992 1993	C	ARG		70 70	32.662 -21.083 25.930 1.00 39.48 30.691 -14.888 20.682 1.00 26.77	В
VT AM	200	_		_		H-1444 H-1111 H-111	

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ATOM	1994	0	ARG		70		-13.725	20.951	1.00 26.95	В
ATOM	1995	N	LYS		71		-15.235	19.608	1.00 25.97	В
ATOM	1996	CA	LYS	В	71	31.885	-14.236	18.670	1.00 25.98	В
MOTA	1997	CB	LYS	В	71	32.830	-14.877	17.652	1.00 27.62	В
ATOM	1998	CG	LYS	В	71	33.728	-13.873	16.924	1.00 29.24	В
MOTA	1999	Ð	LYS	В	71	34.628	-13.137	17.909	1.00 32.14	В
ATOM	2000	CE	LYS		71		-12.035	17.236	1.00 33.13	В
								18.245	1.00 34.18	В
ATOM	2001	NZ	LYS		71		-11.164			
MOTA	2002	C	LYS		71	30.710	-13.591	17.952	1.00 25.22	В
MOTA	2003	0	LYS	В	71	30.719	-12.395	17.671	1.00 24.39	В
MOTA	2004	N	ARG	В	72	29.701	-14.399	17.657	1.00 25.08	В
ATOM	2005	CA	ARG		72	28.500	-13.922	16.989	1.00 26.32	В
ATOM	2006	CB	ARG		72		-15.101	16.561	1.00 28.02	В
									1.00 28.10	В
ATOM	2007	CG	ARG		72		-15.830	15.340		
MOTA	2008	CD	ARG		72	27.225	-17.013	15.083	1.00 32.02	В
MOTA	2009	NB	ARG	В	72	27.451	-17.583	13.766	1.00 36.46	В
ATOM	2010	CZ	ARG	В	72	27.014	-18.779	13.389	1.00 38.62	В
MOTA	2011		ARG	В	72	26.324	-19.538	14.238	1.00 37.88	В
ATOM	2012		ARG		72		-19.212	12.163	1.00 38.55	В
								17.898	1.00 24.31	В
MOTA	2013	C	ARG		72		-13.017			
MOTA	2014	0	ARG		72		-12.326	17.439	1.00 24.84	В
ATOM	2015	N	ALA	В	73	27.990	-13.028	19.189	1.00 26.18	В
ATOM	2016	CA	ALA	В	73	27.267	-12.185	20.140	1.00 28.18	В
MOTA	2017	CB	ALA	В	73	26.973	-12.974	21.418	1.00 28.97	В
MOTA	2018	C	ALA		73	28.056	-10.916	20.472	1.00 28.97	В
						27.528	-9.977	21.066	1.00 30.50	В
MOTA	2019	0	ALA		73 .					
ATOM	2020	N	ALA		74		-10.882	20.070	1.00 29.65	В
ATOM	2021	CA	ALA	В	74	30.170	-9.732	20.347	1.00 30.77	В
ATOM	2022	CB	ALA	В	74	31.558	-9.966	19.764	1.00 30.77	В
MOTA	2023	С	ALA	В	74	29.594	-8.414	19.827	1.00 31.78	В
ATOM	2024	ō	ALA		74	29.789	-7.359	20.438	1.00 32.74	В
					75		-8.465	18.704	1.00 31.60	В
ATOM	2025	N	VAL			28.886				
ATOM	2026	CA	VAL		75	28.308	-7.248	18.145	1.00 32.38	В
ATOM	2027	CB.	VAL	В	75	27.397	-7.539	16.929	1.00 30.51	В
ATOM	2028	CG1	VAL	В	75	27.291	-6.295	16.062	1.00 31.44	В
MOTA	2029	CG2	VAL	В	75	27.931	-8.696	16.137	1.00 33.08	В
ATOM	2030	С	VAL		75	27.465	-6.529	19.201	1.00 33.07	В
							-5.302	19.218	1.00 33.54	В
MOTA	2031	0	VAL		75	27.402				
MOTA	2032	N	ASP		76	26.811	-7.302	20.065	1.00 34.70	В
MOTA	2033	CA	ASP	В	76	25.971	-6.748	21.130	1.00 36.27	В
ATOM	2034	CB	ASP	В	76	24.780	-7.670	21.420	1.00 38.57	В
MOTA	2035	CG	ASP	В	76	23.889	-7.881	20.215	1.00 41.48	В
ATOM	2036		ASP	В	76	23.335	-6.887	19.694	1.00 43.46	В
ATOM	2037	OD2			76	23.739	-9.048	19.792	1.00 43.76	В
							-6.600	22.411	1.00 35.56	В
ATOM	2038	C	ASP		76	26.780				
MOTA	2039	0	ASP		76	26.731	-5.569	23.081	1.00 34.13	В
MOTA	2040	N	ARG	В	7 7	27.508	-7.661	22.744	1.00 35.22	В
MOTA	2041	CA	ARG	В	77	28.343	-7.708	23.937	1.00 34.49	В
MOTA	2042	CB	ARG	В	77	29.071	-9.052	23.991	1.00 37.16	В
MOTA	2043	CG	ARG	В	77	29.841	-9.328	25.271	1.00 40.90	В
ATOM	2044	CD	ARG		77		-10.553	25.102	1.00 43.79	В
			ARG		77		-11.743	24.665	1.00 48.65	В
MOTA	2045	NE								
ATOM	2046	CZ	ARG		77		-12.385	25.406	1.00 51.36	В
ATOM	2047		. ARG		77		-11.949	26.626	1.00 52.34	В
MOTA	2048	NH2	ARG	В	77	28.499	-13.470	24.935	1.00 50.76	В
MOTA	2049	С	ARG	В	77	29.362	-6.576	23.927	1.00 32.18	В
ATOM	2050	0	ARG	В	77	29.499	-5.835	24.896	1.00 32.49	В
MOTA	2051	N	VAI		78	30.073		22.818	1.00 30.66	В
			VAI			31.086		22.707	1.00 29.00	В
MOTA	2052	CA			78					В
MOTA	2053	CB	VAI		78	32.276		21.867	1.00 27.82	
MOTA	2054		L VAI		78	33.327		21.740	1.00 25.08	В
ATOM	2055	CG2	VAI	В	78	32.870	-7.160.	22.504	1.00 23.27	В
MOTA	2056	C	VAI	В	78	30.594	-4.093	22.113	1.00 29.33	В
ATOM	2057	0	VAI	ъв	78	30.435	-3.104	22.831	1.00 29.83	В
ATOM	2058	N	CY		79	30.354		20.804	1.00 28.42	В
		CA		3 B	79	29.927		20.083	1.00 29.14	В
ATOM	2059							20.629	1.00 28.59	В
ATOM	2060	C		3 B	79	28.724				
MOTA	2061	0		B	79	28.883		21.062	1.00 26.06	В
ATOM	2062	CB		5 B	79	29.675		18.604	1.00 29.19	В
ATOM	2063	SG	CY	S B	79	31.052		17.680	1.00 31.71	В
ATOM	2064	N	AR	3 B	80	27.527	-2.693	20.586	1.00 28.34	В
ATOM	2065	CA		3 B	80	26.347		21.071	1.00 30.77	В
ATOM	2066	СВ		3 B	80	25.079		20.915	1.00 32.82	В
		CG		3 B	80			19.474	1.00 35.65	В
ATOM	2067	CG	ALK		60	24.612	4.3/3	17.2/4	2.00 33.03	-

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MOTA	2068	CD	arg	В	80	23.120	-3.273	19.387	1.00 36.01	В
ATOM	2069	NE	ARG	В	80	22.649	-3.243	18.005	1.00 35.49	В
MOTA	2070	CZ	ARG	В	80	22.913	-4.188	17.108	1.00 37.80	В
ATOM	2071		ARG		80	23.640	-5.242	17.449	1.00 40.57	В
ATOM	2072		ARG		80	22.467	-4.075	15.864	1.00 38.86	В
ATOM	2073	С	ARG	В	80	26.507	-1.552	22.524	1.00 31.24	В
MOTA	2074	0	ARG	В	80	25.975	-0.525	22.944	1.00 32.07	В
ATOM	2075	N	HIS		81	27.257	-2.337	23.283	1.00 31.40	В
									1.00 32.20	В
ATOM	2076	CA	HIS		81	27.492	-2.028	24.683		
ATOM	2077	CB	HIS	В	81	28.220	-3.185	25.366	1.00 33.00	B
ATOM	2078	CG	HIS	В	81	28.595	-2.899	26.787	1.00 37.24	В
MOTA	2079		HIS		81	29.764	-2.490	27.335	1.00 38.05	В
							-2.981	27.826	1.00 39.11	В
ATOM	2080		HIS		81	27.692				
MOTA	2081		HIS		81	28.290	-2.635	28.952	1.00 40.49	В
ATOM	2082	NE2	HIS	В	81	29.548	-2.332	28.682	1.00 39.16	В
ATOM	2083	C	HIS	В	81	28.326	-0.762	24.831	1.00 30.87	В
ATOM	2084	ō	HIS		81	27.906	0.206	25.470	1.00 31.38	В
ATOM	2085	N	nra		82	29.511	-0.770	24.233	1.00 29.77	. B
ATOM	2086	CA	asn	В	82	30.403	0.375	24.332	1.00 28.02	В
ATOM	2087	CB	ASN	В	82	31.755	0.056	23.683	1.00 26.64	В
ATOM	2088	CG	ASN		82	32.470	-1.092	24.373	1.00 25.02	В
MOTA	2089		ASN		82	32.305	-1.305	25.572	1.00 24.06	В
ATOM	2090	ND2	ASN	В	82	33.278	-1.829	23.619	1.00 26.38	В
ATOM	2091	C	ASN	В	82	29.819	1.648	23.741	1.00 26.04	В
ATOM	2092	ō	ASN		82	30.163	2.747	24.174	1.00 25.71	В
									1.00 25.90	В
MOTA	2093	N	TYR		83	28.930	1.512	22.765		
MOTA	2094	CA	TYR	В	83	28.324	2.693	22.156	1.00 25.91	В
ATOM	2095	CB	TYR	В	83	27.462	2.297	20.946	1.00 25.69	В
ATOM	2096	CG	TYR		83	27.102	3.462	20.056	1.00 25.95	В
							4.294	20.353	1.00 27.11	В
ATOM	2097		TYR		83	26.022				
MOTA	2098	CE1	TYR	В	83	25.712	5.403	19.545	1.00 25.98	В
MOTA	2099	CD2	TYR	В	83	27.865	3.759	18.933	1.00 27.72	В
ATOM	2100	CE2	TYR	В	83	27.567	4.862	18.121	1.00 28.05	В
	2101	CZ	TYR		83	26.493	5.680	18.434	1.00 27.73	В
MOTA										В
MOTA	2102	OH	TYR		83	26.225	6.781	17.645	1.00 27.55	
ATOM	2103	С	TYR	В	83	27.485	3.458	23.181	1.00 25.87	В
MOTA	2104	0	TYR	В	83	27.315	4.673	23.070	1.00 26.05	В
MOTA	2105	N	GLN		84	26.975	2.750	24.186	1.00 28.25	В
							3.375	25.229	1.00 30.44	В
MOTA	2106	CA	GLN		84	26.159				
MOTA	2107	CB	GLN	В	84	25.467	2.310	26.093	1.00 34.30	В
MOTA	2108	CG	GLN	В	84	24.595	1.343	25.301	1.00 40.52	В
ATOM	2109	CD	GLN	В	84	23.515	2.047	24.496	1.00 43.21	В
ATOM	2110		GLN		84	23.023	1.516	23.499	1.00 46.12	В
										В
MOTA	2111		GLN		84	23.133	3.244	24.932	1.00 45.41	
MOTA	2112	C	GLIN	В	84	27.030	4.254	26.111	1.00 29.01	В
MOTA	2113	0	GLIN	В	84	26.633	5.353	26.494	1.00 27.82	В
MOTA	2114	N	LEU	r B	85	28.219	3.757	26.436	1.00 28.32	В
							4.505	27.263		В
MOTA	2115	CA	LEU		85	29.150				
MOTA	2116	CB	LEU	B	85	30.355	3.631	27.631	1.00 28.92	В
MOTA	2117	CG	LEU	B	85	30.065	2.226	28.184	1.00 30.98	В
ATOM	2118	CD1	LEU	В	85	31.343	1.631	28.758	1.00 30.59	В
MOTA	2119	-	LEU		85	29.006	2.291	29.265	1.00 31.87	В
							5.719	26.461	1.00 29.95	В
MOTA	2120	C	LEU		85	29.609				
MOTA	2121	0	LEU		85	29.836	6.798	27.010	1.00 30.93	В
MOTA	2122	N	GLU	JB	86	29.724	5.529	25.150	1.00 30.31	В
MOTA	2123	CA	GLU	B	86	30.160	6.577	24.245	1.00 31.41	В
MOTA	2124	CB	· GLU		86	30.426	5.981	22.861	1.00 32.60	В
								22.236	1.00 39.25	В
MOTA	2125	CG	GL		86	31.741	6.420			
MOTA	2126	CD	GLU	JВ	86	32,962	5.854	22.953	1.00 41.02	В
MOTA	2127	OE:	L GLU	JB	86	33.379	4.714	22.636	1.00 40.75	В
ATOM	2128	OE:	GLT	J B	86	33.497	6.553	23.843	1.00 41.96	В
						29.113	7.684	24.146	1.00 32.44	В
MOTA	2129	C	GLU		86					
MOTA	2130	0	GLU		86	29.454	8.865	24.109	1.00 30.73	В
ATOM	2131	N	TRI	JB	87	27.838	7.303	24.103	1.00 33.77	В
ATOM	2132	CA	LEU		87	26.755	8.282	24.015	1.00 34.65	В
-	2133	СВ	LEG		87	25.398	7.583	23.899	1.00 34.69	В
MOTA										В
ATOM	2134	CG		JB	87	24.916	7.169	22.508	1.00 36.86	
ATOM	2135	CD:	1 LE	JB	87	23.655	6.326	22.642	1.00 35.43	В
ATOM	2136	CD	2 LET	JB	87	24.645	8.411	21.660	1.00 35.76	В
ATOM	2137	C		J B	87	26.740	9.199	25.231	1.00 35.16	В
	2138	ō		UB	87	26.250	10.326	25.164	1.00 34.29	В
MOTA									1.00 36.69	В
MOTA	2139			G B		27.280	8.711	26.343		
MOTA	2140			3 B		27.317	9.493	27.573	1.00 37.64	В
MOTA	2141	CB	AR	G B	88	27.173	8.575	28.791	1.00 39.79	В

ATOM	2142	CG	ARG	В	88	25.827	7.878	28.908	1.00 45.19	В
ATOM	2143	CD	ARG	В	88	25.704	7.173	30.253	1.00 49.04	В
MOTA	2144	NE	ARG	В	88	26.657	6.074	30.388	1.00 54.57	В
MOTA	2145	CZ	ARG	В	88	27.101	5.603	31.552	1.00 55.76	В
ATOM	2146		ARG		88	26.683	6.137	32.694	1.00 55.56	В
ATOM	2147	NH2	ARG		88	27.963	4.595	31.574	1.00 56.11	В
ATOM	2148	C	ARG		88	28.601	10.299	27.714	1.00 36.93	В
ATOM	2149	ō	ARG		88	28.702	11.160	28.589	1.00 37.24	В
ATOM	2150	Ŋ	THR		89	29.571	10.035	26.842	1.00 35.19	В
ATOM	2151	CA	THR		89	30.860	10.712	26.914	1.00 31.71	В
ATOM			THR		89	31.916	9.767	27.529	1.00 31.71	В
	2152	CB CC1					8.554	26.762	1.00 31.01	
MOTA	2153		THR		89	31.980				В
ATOM	2154		THR		89	31.557	9.436	28.963	1.00 25.87	В
ATOM	2155	C	THR		89	31.420	11.254	25.600	1.00 31.31	В
MOTA	2156	0	THR		89	31.214	12.415	25.249	1.00 32.41	В
ATOM	2157	N	THR		90	32.139	10.403	24.880	1.00 30.72	В
ATOM	2158	CA	THR		90	32.766	10.786	23.623	1.00 30.43	В
ATOM	2159	CB	THR		90	33.368	9.558	22.925	1.00 30.54	В
ATOM	2160		THR		90	34.297	8.919	23.808	1.00 33.70	В
MOTA	2161	CG2	THR		90	34.099	9.970	21.666	1.00 31.65	В
ATOM	2162	С	THR	В	90	31.874	11.512	22.625	1.00 30.61	, B
ATOM	2163	0	THR	В	90	32.267	12.543	22.070	1.00 30.24	В
MOTA	2164	N	TRO	В	91	30.683	10.977	22.385	1.00 30.30	В
ATOM	2165	CA	LEU	В	91	29.767	11.581	21.425	1.00 31.93	В
ATOM	2166	CB	LEU	В	91	28.709	10.554	21.007	1.00 32.55	В
ATOM	2167	CG	PEA	В	91	29.268	9.315	20.292	1.00 33.01	В
ATOM	2168	CD1	LEU	В	91	28.201	8.233	20.205	1.00 33.73	В
ATOM	2169	CD2	LEU	В	91	29.761	9.700	18.902	1.00 31.26	В
ATOM	2170	C	LEU		91	29.096	12.872	21.907	1.00 32.38	В
ATOM	2171	ō	LEU		91	28.402	13.534	21.139	1.00 32.08	В
ATOM	2172	N	GLN		92	29.303	13.229	23.173	1.00 32.44	В
ATOM	2173	CA	GLN		92	28.725	14.454	23.713	1.00 34.54	В
ATOM	2174	CB	GLN		92	28.138	14.217	25.110	1.00 38.48	В
MOTA	2175	CG	GLN		92	26.836	13.419	25.121	1.00 44.66	В
		CD CD	GLN		92	26.233	13.291	26.516	1.00 49.27	В
ATOM	2176									В
ATOM	2177	OB1			92	25.239	12.588	26.712	1.00 51.65	
MOTA	2178	NE2	GLN		92	26.832	13.975	27.491	1.00 49.93	. B
MOTA	2179	C	GLN		92	29.779	15.557	23.777	1.00 32.86	' В
MOTA	2180	0	GLN		92	29.457	16.721	24.019	1.00 32.19	В
MOTA	2181	N	ARG		93	31.038	15.187	23.555	1.00 31.53	В
ATOM	2182	CA	ARG		93	32.132	16.157	23.576	1.00 29.87	В
ATOM	2183	CB	ARG	В	93	33.477	15.472	23.302	1.00 28.14	В
ATOM	2184	CG	ARG		93	34.681	16.433	23.217	1.00 23.56	В
ATOM	2185	CD	ARG	В	93	35.953	15.656	22.925	1.00 22.53	В
ATOM	2186	NE	ARG	В	93	37.128	16.486	22.662	1.00 19.19	В
MOTA	2187	CZ	ARG	В	93	37.769	17.205	23.581	1.00 18.66	В
ATOM	2188	NH1	ARG	В	93	37.352	17.214	24.843	1.00 17.45	В
ATOM	2189	NH2	ARG	В	93	38.847	17.898	.23.242	1.00 16.56	В
MOTA	2190	С	ARG	В	93	31.921	17.245	22.535	1.00 29.02	В
ATOM	2191	0	ARG	В	93	31.755	16.965	21.349	1.00 29.55	В
MOTA	2192	N	ARG	В	94	31.933	18.490	22.987	1.00 28.71	В
ATOM	2193	CA	ARG	В	94	31.767	19.613	22.087	1.00 29.63	В
MOTA	2194	CB	ARG	В	94	30.299	20.046	22.041	1.00 32.44	B
MOTA	2195	CG	ARG		94	29.506	19.196	21.060	1.00 37.10	В
ATOM	2196	CD	ARG		94	28.016	19.414	21,124	1.00 39.80	В
ATOM	2197	NE	ARG		94	27.350	18.742	20.008	1.00 44.04	В
ATOM	2198	CZ	ARG		94	27.372	17.428	19.791	1.00 44.11	В
ATOM	2199		ARG		94	28.026	16.625	20.617	1.00 45.60	В
ATOM	2200		ARG		94	26.747	16.916	18.739	1.00 44.45	В
ATOM	2201	C	ARG		94	32.656		. 22.498	1.00 28.84	В
	2202	0	ARG		94	32.464	21.363	23.550	1.00 20.04	В
ATOM	2202						21.038	21.663	1.00 27.49	В
MOTA		N	VAL		95	33.650				
ATOM	2204	CA	VAL		95 05	34.592	22.117	21.916	1.00 26.47	В
MOTA	2205	CB	VAL		95	36.047	21.605	21.890	1.00 25.65	В
ATOM	2206		. VAL		95	37.004	22.734	22.260	1.00 22.82	В
MOTA	2207		VAL		95	36.202	20.423	22.849	1.00 26.01	В
MOTA	2208	С	VAL		95	34.415	23.180	20.840	1.00 27.00	В
MOTA	2209	0	VAL		95	34.721	22.945	19.665	1.00 27.00	В
MOTA	2210	N	GLU		96	33.912	24.340	21.253	1.00 26.94	В
MOTA	2211	CA	GLU		96	33.673	25.462	20.348	1.00 26.50	В
ATOM	2212	CB	GTO		96	33.072	26.649	21.107	1.00 29.19	В
MOTA	2213	CG	GLU	В	96	31.736	26.372	21.775	1.00 36.47	В
MOTA	2214	CD	GLU	В	96	31.211	27.582	22.537	1.00 40.45	В
MOTA	2215	OE:	GLU	В	96	30.121	27.477	23.144	1.00 42.85	В

MOTA 2216 OE2 GLU B 96 31.891 28.634 22.526 1.00 40.11 В GLU B 96 34.960 25.916 19.689 1.00 25.02 MOTA 2217 C 35,999 26.022 20.338 1.00 24.73 MOTA 2218 0 GLU B 96 MOTA 2219 N PRO B 97 34.900 26.204 18.383 1.00 24.54 MOTA 2220 CD PRO B 97 33.744 26.011 17,493 1.00 22.89 PRO B 97 36.069 26.655 17.626 1.00 23.87 CA MOTA 2221 35.580 26.633 16.175 1.00 22.81 MOTA 2222 CB PRO B 97 PRO B 97 34.411 25.663 16.202 1.00 25.55 MOTA 2223 CG 1.00 23.80 MOTA C PRO B 97 36.498 28.061 18.021 2224 35.665 28.905 18.353 1.00 24.40 PRO B 97 ATOM 2225 0 37.799 1.00 22.02 ATOM 2226 N THR B 98 28,307 17.990 В ATOM 2227 CA THR B 98 38.306 29.634 18.266 1.00 24.00 В THR B 98 39.569 29.592 19.150 1.00 27.31 ATOM 2228 CB 40.626 28.929 18.449 1.00 35.69 В ATOM 2229 OG1 THR B 98 1.00 26.76 MOTA 2230 CG2 THR B 98 39.282 28.839 20.439 38.631 30.143 16.860 1.00 22.38 В MOTA 2231 C THR B 98 THR B 98 39.376 29.504 16.116 1.00 19.48 В ATOM 2232 0 1.00 21.55 VAL B 99 38.041 31.274 16.487 ATOM 2233 N 15.152 1.00 21.20 2234 CA VAL B 99 38.242 31.824 В MOTA VAL B 99 36.871 32.153 14.509 1.00 21.09 R MOTA 2235 CB CG1 VAL B 99 37.043 32.541 13.050 1.00 19.62 MOTA 2236 35.950 30.944 14.625 1.00 18.29 CG2 VAL B 99 MOTA 2237 15.167 1.00 21.59 2238 VAL B 99 39.140 33.059 В MOTA C VAL B 99 38.970 33.962 15.982 1.00 21.57 В ATOM 2239 0 1.00 22.65 THR B 100 40.099 33.084 14.252 MOTA 2240 N 41.056 14.168 1.00 24.95 34.179 ATOM 2241 CA THR B 100 14.820 1.00 26.31 THR B 100 42.399 33.770 В MOTA 2242 CB MOTA 2243 OG1 THR B 100 42.162 33.321 16.160 1.00 30.10 В 43.359 34.942 14.854 1.00 29.07 CG2 THR B 100 MOTA 2244 41.329 34.556 12.717 1.00 24.61 MOTA 2245 C THR B 100 MOTA 2246 THR B 100 41.514 33.689 11.869 1.00 23.89 ILE B 101 41.363 35.852 12.435 1.00 26.18 2247 MOTA N 36.315 11.080 1.00 29.32 41.638 MOTA 2248 CA ILE B 101 1.00 29.37 40.572 37.327 10.582 ATOM 2249 CB ILE B 101 9.231 1.00 29.49 ATOM 2250 CG2 ILE B 101 40.986 37.885 10.492 1.00 30.11 CG1 ILE B 101 39.198 36.664 ATOM 2251 10.002 1.00 29.81 CD1 ILE B 101 38.110 37.605 ATOM 2252 42.988 37.015 11.040 1.00 31.04 2253 ILE B 101 MOTA С ILE B 101 43.270 37.868 11.877 1.00 31.24 В MOTA 2254 0 43.820 36.664 10.066 1.00 34.47 SER B 102 MOTA 2255 N 45.124 37.303 9.940 1.00 39.17 MOTA 2256 CA SER B 102 1.00 37.33 2257 CB **SER B 102** 46.143 36.617 10.844 ATOM 46.326 35.265 10.462 1.00 41.93 B MOTA 2258 OG **SER B 102** SER B 102 45.632 37.289 8.501 1.00 42.45 В C ATOM 2259 45.641 36.248 7.845 1.00 42.45 **SER B 102** ATOM 2260 0 46.052 38.455 7.988 1.00 45.38 В PRO B 103 ATOM 2261 45.938 39.793 8.596 1.00 45.47 В MOTA 2262 CD PRO B 103 1.00 48.91 В PRO B 103 46.564 38.545 6.617 ATOM 2263 CA 46.446 40.032 6.312 1.00 47.74 В ATOM 2264 CB PRO B 103 1.00 47.08 46.739 40.652 7.642 2265 PRO B 103 ATOM CG 1.00 51.96 В MOTA 2266 C PRO B 103 48.010 38.042 6.545 48.688 37.957 7.568 1.00 52.51 В ATOM 2267 0 PRO B 103 SER B 104 48.475 37.699 5.346 1.00 55.84 MOTA 2268 N 1.00 60.00 49.843 37.209 5.177 MOTA 2269 CA **SER B 104** 1.00 59.60 **SER B 104** 50.018 36.578 3.791 ATOM 2270 CB OG **SER B 104** 49.778 37.520 2.759 1.00 59.05 ATOM 2271 50.842 38.353 5.368 1.00 63.75 В SER B 104 MOTA C 2272 50.853 39.325 1.00 64.64 4.605 ATOM 2273 ٥ SER B 104 1.00 66.99 51.677 ATOM 2274 N ARG B 105 38.228 6.398 52.674 39.242 6.736 1.00 69.17 В MOTA 2275 CA ARG B 105 1.00 70.33 53.631 38.700 7.808 ARG B 105 ATOM 2276 CB 37.690 1.00 72.24 54.672 7.318 MOTA 2277 CG ARG B 105 54.073 36.586 6.449 1.00 73.51 MOTA 2278 œ ARG B 105 52.981 35.859 7.095 1.00 75.02 В ARG B 105 MOTA NE 2279 В ARG B 105 53.120 35.051 8.142 1.00 76.07 ATOM 2280 CZ 1.00 77.38 ATOM 2281 NH1 ARG B 105 54.314 34.852 8.684 1.00 76.05 ATOM 2282 NH2 ARG B 105 52.059 34.431 8.644 В 53.464 39.720 5.523 1.00 70.38 ARG B 105 ATOM 2283 C В 53.134 40.746 4.923 1.00 71.56 ATOM 2284 0 ARG B 105 1.00 49.25 R 46.629 40.478 -1.867 MOTA 2285 **ASN B 113** N 1.00 48.42 **ASN B 113** 46.963 40.039 -0.515 ATOM 2286 CA 46.726 41.181 0.477 1.00 51.23 ATOM 2287 CB **ASN B 113** 1.00 53.89 В ASN B 113 47.268 40.875 1.863 ATOM CG 2288 48.429 40.498 2.019 1.00 55.14 MOTA 2289 OD1 ASN B 113

MOTA	2290	ND2	ASN E	113	46.428	41.048	2.880	1.00 55.30	В
MOTA	2291	C	ASN E	113	46.143	38.808	-0.118	1.00 45.78	В
ATOM	2292	ō	ASN E		45.155	38.471	-0.774	1.00 44.99	В
MOTA	2293	N	TEO E		46.550	38.146	0.961	1.00 42.27	В
MOTA	2294	CA	TEO E		45.862	36.944	1.415	1.00 38.77	В
ATOM	2295	CB	LEU E	114	46.770	35.739	1.182	1.00 39.10	В
ATOM	2296	CG	TEA E	114	46.238	34.330	1.421	1.00 40.81	В
ATOM	2297	CD1	LEU E	114	45.097	34.023	0.459	1.00 41.59	В
ATOM	2298	CD2	LEU E	3 114	47.379	33.341	1.222	1.00 41.03	В
MOTA	2299	C	LEU E		45.424	36.986	2.883	1.00 36.39	В
ATOM		ŏ					3.783	1.00 35.98	В
	2300		LEU E		46.237	37.204			
ATOM	2301	N	LEU E		44.130	36.777	3.112	1.00 31.79	В
MOTA	2302	CA	TEO E		43.576	36.766	4.460	1.00 28.77	В
ATOM	2303	CB	TEA E	3 115	42.231	37.496	4.493	1.00 29.52	В
ATOM	2304	CG	LEU E	3 115	42.156	38.843	5.218	1.00 30.12	В
ATOM	2305	CD1	LEU E	3 115	43.281	39.751	4.764	1.00 30.28	В
ATOM	2306	CD2	TEO E		40.799	39.479	4.951	1.00 28.39	В
ATOM	2307	c	LEU E		43.374	35.323	4.896	1.00 27.23	В
ATOM	2308	0	LEU E		42.815	34.513	4.154	1.00 25.72	В
ATOM	2309	N	VAL E		43.825	35.002	6.103	1.00 24.13	В
MOTA	2310	CA	VAL E		43.695	33.651	6.618	1.00 20.76	В
MOTA	2311	CB	VAL E	3 116	45.078	33.098	7.078	1.00 20.02	В
ATOM	2312	CG1	VAL E	3 116	44.915	31.757	7.777	1.00 17.46	В
ATOM	2313	CG2	VAL E	3 116	45.996	32.944	5.880	1.00 19.44	В
ATOM	2314	c	VAL I		42.723	33.568	7.784	1.00 20.38	В
			VAL I			34.293	8.766	1.00 19.54	В
ATOM	2315	0			42.860				
ATOM	2316	N	CYS I		41.724	32.701	7.669	1.00 20.87	В
MOTA	2317	CA	CYS I		40.793	32.523	8.774	1.00 22.57	В
MOTA	2318	C	CYS I	3 117	41.132	31.196	9.444	1.00 21.84	В
ATOM	2319	0	CYS I	3 117	40.867	30.123	8.892	1.00 22.98	В
MOTA	2320	CB	CYS I	3 117	39.332	32.486	8.315	1.00 23.53	В
ATOM	2321	SG	CYS I		38.217	32.222	9.734	1.00 29.76	В
ATOM	2322	N	SER I		41.728	31.277	10.627	1.00 19.87	В
			SER I		42.094	30.092	11.381	1.00 18.65	В
MOTA	2323	CA							
MOTA	2324	CB	SER I		43.345	30.356	12.226	1.00 19.67	В
MOTA	2325	OG	SER I		44.463	30.672	11.421	1.00 22.97	В
ATOM	2326	С	SER I	3 118	40.962	29.656	12.300	1.00 18.03	В
ATOM	2327	0	SER I	3 118	40.579	30.389	13.209	1.00 19.82	В
MOTA	2328	N	VAL I	B 119	40.426	28.463	12.050	1.00 17.57	В
ATOM	2329	CA	VAL 1		39.365	27.889	12.874	1.00 15.30	В
MOTA	2330	СВ	VAL		38.202	27.364	12.006	1.00 15.69	В
ATOM			VAL		37.091	26.852	12.892	1.00 11.64	В
	2331								В
ATOM	2332		VAL 1		37.695	28.484	11.076	1.00 13.82	
MOTA	2333	С	VAL		40.073	26.739	13.579	1.00 15.38	В
MOTA	2334	0	VAL	B 119	40.318	25.680	12.992	1.00 16.76	В
MOTA	2335	N	THR 1	B 120	40.404	26.958	14.844	1.00 16.03	В
ATOM	2336	CA	THR I	B 120	41.165	25.988	15.615	1.00 15.04	В
MOTA	2337	CB	THR I	B 120	42.487	26.613	16.031	1.00 13.75	В
ATOM	2338		THR :		42.221	27.713	16.915	1.00 17.84	В
ATOM	2339	CG2		B 120	43.230	27.144	14.815	1.00 12.18	В
		C		B 120	40.533	25.405	16.872	1.00 17.87	В
MOTA	2340								В
MOTA	2341	0		B 120	39.571	25.944	17.425	1.00 17.71	
MOTA	2342	N		B 121	41.132	24.303	17.317	1.00 19.07	В
ATOM	2343	CA	ASP :	B 121	40.738	23.576	18.511	1.00 20.97	В
MOTA	2344	CB	ASP :	B 121	41.268	24.291	19.766	1.00 24.82	В
MOTA	2345	CG	ASP :	B 121	42.797	24.330	19.831	1.00 31.04	В
MOTA	2346	OD1	ASP :	B 121	43.460	23.360	19.397	1.00 30.81	В
MOTA	2347		ASP		43.339	25.333	20.346	1.00 34.38	В
MOTA	2348	C		B 121	39.238	23.293	18.679	1.00 21.27	В
ATOM				B 121	38.629	23.671	19.683	1.00 23.00	В
	2349	0							В
MOTA	2350	N		B 122	38.641	22.613	17.710	1.00 20.38	
ATOM	2351	ÇA		B 122	37.233	22.280	17.818	1.00 18.51	В
MOTA	2352	CB	PHE	B 122	36.414	22.988	16.732	1.00 16.18	В
ATOM	2353	CG	PHE	B 122	36.817	22.644	15.319	1.00 13.31	В
MOTA	2354		PHE		37.695	23.463	14.615	1.00 11.43	В
ATOM	2355		PHE		36.247	21.547	14.664	1.00 10.93	В
ATOM	2356		PHE		37.998	23.210	13.272	1.00 10.91	В
					36.541	21.280	13.317	1.00 12.31	В
MOTA	2357		PHE						В
ATOM	2358	CZ		B 122	37.419	22.118	12.618	1.00 8.92	
MOTA	2359	С		B 122	37.011	20.778	17.739	1.00 19.55	В
MOTA	2360	0		B 122	37.889	20.029	17.301	1.00 18.45	В
ATOM	2361	N	TYR	B 123	35.829	20.357	18.182	1.00 20.50	В
ATOM	2362	CA	TYR	B 123	35.412	18.959	18.180	1.00 21.08	В
ATOM	2363	CB		B 123	36.067	18.201	19.340	1.00 19.11	В

ATOM	2364	CG	TYR B	123	35.919	16.702	19.228	1.00 18.56	В
ATOM	2365		TYR B		34.746	16.062	19.629	1.00 19.13	В
MOTA	2366		TYR B		34.572	14.695	19.446	1.00 17.75	В
MOTA	2367	CD2	TYR B	123	36.920	15.932	18.647	1.00 17.20	В
ATOM	2368	CE2	TYR B	123	36.762	14,566	18.455	1.00 17.38	В
		cz	TYR B		35.584	13.953	18.853	1.00 19.59	В
MOTA	2369								
MOTA	2370	ОН	TYR B	123	35.412	12.608	18.631	1.00 22.32	В
MOTA	2371	С	TYR B	123	33.896	18.957	18.351	1.00 21.83	В
									В
MOTA	2372	0	TYR B		33.365	19.708	19.165	1.00 23.26	
ATOM	2373	N	PRO B	124	33.175	18.126	17.584	1.00 21.65	В
MOTA	2374	æ	PRO B	124	31.725	17.996	17.808	1.00 23.81	В
ATOM		CA	PRO B		33.627	17.177	16.562	1.00 22.30	В
	2375								
MOTA	2376	СВ	PRO B	124	32.398	16.290	16.353	1.00 21.95	В
ATOM	2377	CG	PRO B	124	31.270	17.237	16.586	1.00 23.07	В
ATOM	2378	C	PRO B	124	34.128	17.813	15.266	1.00 22.20	В
			PRO B					1.00 24.43	В
ATOM	2379	0			34.204	19.035	15.149		
ATOM	2380	N	ALA B	125	34.457	16.971	14.291	1.00 20.63	В
ATOM	2381	CA	ALA B	125	34.987	17.428	13,007	1.00 22.13	В
MOTA	2382	CB	ALA B		35.571	16.236	12.244	1.00 20.20	В
MOTA	2383	C	ALA B	125	34.057	18.222	12.078	1.00 22.42	В
MOTA	2384	0	ALA B	125	34.512	19.129	11.400	1.00 24.48	В
ATOM	2385	N	GLN B	126	32.772	17.893	12.036	1.00 25.59	В
									В
ATOM	2386	CA	GLN B		31.845	18.598	11.147	1.00 27.46	
ATOM	2387	CB	GLN B	126	30.414	18.101	11.357	1.00 29.99	В
MOTA	2388	CG	GLN B	126	30.283	16.595	11.480	1.00 36.21	В
		CD	GLN B		30.625	16.102	12.870	1.00 38.28	В
ATOM	2389								
MOTA	2390	OE1	GITM E	126	30.558	14.905	13.158	1.00 40.46	В
ATOM	2391	NE2	GLN E	126	30.989	17.030	13.745	1.00 40.92	В
ATOM	2392	C	GLN E	126	31.876	20.112	11.333	1.00 28.28	В
MOTA	2393	0	GLN E	126	31.571	20.627	12.410	1.00 29.36	В
MOTA	2394	N	ILE E	127	32.221	20.831	10.273	1.00 27.17	В
ATOM	2395	CA	ILE E	127	32.292	22.279	10.353	1.00 27.02	В
			ILE E			22.716	10.931	1.00 27.21	В
ATOM	2396	CB			33.656				
ATOM	2397	CG2	ILE E	127	34.767	22.453	9.898	1.00 21.63	В
MOTA	2398	CG1	ILE F	3 127	33.612	24.195	11.316	1.00 24.63	В
ATOM	2399		ILE E		34.760	24.633	12.198	1.00 25.86	В
ATOM	2400	C	IFE E	127	32.117	22.903	8.969	1.00 27.10	В
ATOM	2401	0	ILE E	3 127	32.393	22.258	7.956	1.00 26.58	В
ATOM	2402	N	LYS E	3 128	31.666	24.155	8.940	1.00 25.41	В
							7.689	1.00 27.45	В
ATOM	2403	CA	LYS E		31.457	24.884			
MOTA	2404	CB	LYS E	3 128	29.964	24.927	7.334	1.00 29.68	В
MOTA	2405	CG	LYS F	3 128	29.633	25.685	6.046	1.00 34.69	В
		CD	LYS E		30.129	24.954	4.793	1.00 38.25	В
ATOM	2406								
ATOM	2407	CE	LYS E		29.802	25.742	3.517	1.00 40.20	В
ATOM	2408	NZ	LYS I	3 128	30.281	25.071	2.271	1.00 39.87	В
MOTA	2409	C	LYS I	3 128	31.983	26.301	7.861	1.00 25.41	В
						27.019	8.759	1.00 26.68	В
MOTA	2410	0	LYS I		31.559				
MOTA	2411	N	VAL I	3 129	32.911	26.700	7.002	1.00 25.70	В
MOTA	2412	CA	VAL I	3 129	33.493	28.034	7.078	1.00 24.82	В
ATOM	2413	СВ	VAL I	3 129	35.013	27.956	7.329	1.00 24.17	В
								1.00 22.14	В
ATOM	2414		VAL I		35.592	29.351	7.452		
ATOM	2415	CG2	VAL 1	3 129	35.295	27.136	8.583	1.00 22.44	В
MOTA	2416	С	VAL I	B 129	33.248	28.791	5.778	1.00 25.17	В
ATOM	2417	0		3 129	33.532	28.283	4.701	1.00 25.50	В
								1.00 27.21	В
MOTA	2418	N		B 130	32.724	30.007	5.884		
MOTA	2419	ÇA	ARG 1	B 130	32.445	30.814	4.701	1.00 28.49	В
ATOM	2420	CB	ARG 1	B 130	30.931	30.920	4.470	1.00 31.77	В
				B 130	30.239	29.591	4.183	1.00 34.92	В
ATOM	2421	CG	-						
MOTA	2422	CD	ARG !	B 130	28.927	29.813	3.432	1.00 41.30	В
ATOM	2423	NE	ARG 1	B 130	27.834	30.254	4.291	1.00 42.15	В
ATOM	2424	CZ		B 130	27.032	29.426	4.953	1.00 46.05	В
									В
MOTA	2425	NH	L ARG	B 130	27.200	28.112	4.849	1.00 45.50	
MOTA	2426	NH2	ARG :	B 130	26.061	29.910	5.718	1.00 48.30	В
ATOM	2427	C		B 130	33.036	32.211	4.792	1.00 27.57	В
				B 130	33.130	32.789	5.874	1.00 26.00	В
ATOM	2428	0							
MOTA	2429	N		B 131	33.440	32.744	3.645	1.00 27.37	В
ATOM	2430	CA	TRP	B 131	34.004	34.085	3.571	1.00 30.27	В
ATOM	2431	CB		B 131	35.281	34.083	2.737	1.00 30.21	В
								1.00 32.32	В
MOTA	2432	CG		B 131	36.532	33.844	3.521		
MOTA	2433	CD:	TRP	B 131	37.155	34.757	4.432	1.00 32.41	В
ATOM	2434	CE	TRP	B 131	38.334	34.142	4.900	1.00 33.07	В
ATOM	2435		TRP		36.831	36.039	4.897	1.00 31.75	В
								1.00 32.80	В
ATOM	2436		l TRP		37.333	32.741	3.478		
ATOM	2437	NE:	1 TRP	B 131	38.420	32.913	4.300	1.00 31.53	В

MOTA	2438	CZ2	TRP B	131	39.193	34.764	5.812	1.00 32.82	В
ATOM	2439	CZ3	TRP B		37.680	36.656	5.800	1.00 32.08	В
MOTA	2440		TRP B		38.849	36.017	6.249	1.00 33.40	В
ATOM	2441	C	TRP B		33.003	35.064	2.949	1.00 32.99	В
ATOM	2442	0	TRP B		32.367	34.759	1.940	1.00 32.18	В
ATOM	2443	N	PHE B		32.879	36.242	3.550	1.00 35.48	В
MOTA MOTA	2444 2445	CA CB	PHE B		31.962 30.856	37.263 37.501	3.058 4.077	1.00 39.35	B B
ATOM	2446	CG	PHE B		29.843	36.407	4.123	1.00 38.39	В
MOTA	2447		PHE B		28.804	36.373	3.202	1.00 38.31	В
ATOM	2448		PHE B		29.930	35.399	5.075	1.00 38.21	В
ATOM	2449		PHE B		27.860	35.348	3.229	1.00 39.26	В
ATOM	2450		PHE B		28.992	34.369	5.111	1.00 38.83	В
ATOM	2451	CZ	PHE B	132	27.954	34.345	4.184	1.00 37.91	В
MOTA	2452	C	PHE B	132	32.650	38.583	2.755	1.00 41.59	В
MOTA	2453	0	PHE B		33.515	39.025	3.508	1.00 42.72	В
MOTA	2454	N	ARG B		32.267	39.203	1.640	1.00 45.04	В
ATOM	2455	CA	ARG B		32.829	40.490	1.242	1.00 48.28	В
MOTA	2456	СВ	ARG B		32.510	40.787	-0.227	1.00 51.68	В
ATOM	2457	CG	ARG B		33.293	41.958	-0.829	1.00 55.78	B B
ATOM	2458	CD NE	ARG B		34.787 35.580	41.655 42.741	-0.867 -1.440	1.00 57.07 1.00 59.30	В
ATOM ATOM	2459 2460	CZ	ARG B		35.523	43.135	-2.710	1.00 60.93	В
ATOM	2461		ARG B		34.702	42.536	-3.564	1.00 61.44	В
ATOM	2462		ARG B		36.295	44.132	-3.128	1.00 61.77	В
ATOM	2463	c	ARG B		32.129	41.492	2.145	1.00 49.07	В
ATOM	2464	ō	ARG B		32.299	41.460	3.358	1.00 51.26	В
ATOM	2465	N	ASN B	134	31.331	42.376	1.572	1.00 49.23	В
MOTA	2466	CA	ASN B	134	30.614	43.336	2.393	1.00 48.83	В
ATOM	2467	CB	asn b		30.582	44.702	1.710	1.00 45.93	В
ATOM	2468	CG	asn b		31.973	45.290	1.523	1.00 45.10	В
MOTA	2469		asn b		32.450	45.440	0.397	1.00 41.81	В
ATOM	2470		ASN B		32.634	45.618	2.634	1.00 41.82	В
ATOM	2471	C	ASN B		29.203	42.795	2.594	1.00 50.25 1.00 52.28	B B
ATOM ATOM	2472 2473	N O	ASN B		28.222 29.122	43.529 41.496	2.508 2.868	1.00 52.28	В
MOTA	2474	CA.	ASP B		27.847	40.819	3.072	1.00 51.07	В
ATOM	2475	C	ASP B		27.590	39.855	1.910	1.00 51.76	В
ATOM	2476	ō	ASP B		26.586	39.136	1.893	1.00 51.82	В
ATOM	2477	N	GLN B	136	28.507	39.856	0.944	1.00 50.97	В
MOTA	2478	CA	GLN B	136	28.421	38.999	-0.240	1.00 51.24	В
ATOM	2479	CB	GLN B		28.766	39.805	-1.493	1.00 53.78	В
MOTA	2480	CG	GLN B		28.736	39.000	-2.783	1.00 58.16	В
MOTA	2481	CD	GLN B		29.675	39.559	-3.839 -3.675	1.00 59.39 1.00 60.12	B B
ATOM ATOM	2482 2483	NE2	GLN B		30.895 29.110	39.527 40.078	-4.926	1.00 59.45	В
ATOM	2484	C	GLN B		29.395	37.825	-0.124	1.00 49.46	В
ATOM	2485	ō	GLN B		30.607	38.026	-0.035	1.00 48.29	В
MOTA	2486	N	GLU E		28.873	36.603	-0.144	1.00 47.64	В
ATOM	2487	CA	GLU E		29.730	35.432	-0.027	1.00 46.85	В
MOTA	2488	СВ	GLU E	137	28.899	34.152	0.022	1.00 47.17	В
MOTA	2489	CG	GLU E	137	29.695	32.975	0.556	1.00 50.22	В
MOTA	2490	CD	GLU E		28.866	31.726	0.743	1.00 52.65	В
MOTA	2491		GLU E		27.699	31.842	1.171	1.00 55.57	В
MOTA	2492		GLU E		29.391	30.623	0.478	1.00 54.41	В
ATOM	2493	C	GLU F		30.755	35.320	-1.149	1.00 45.23 1.00 45.04	B B
MOTA	2494	0	GLU E		30.445 31.983	35.544 34.977	-2.314 -0.776	1.00 44.63	В
ATOM ATOM	2495 2496	N CA	GLU E		33.078	34.808	-1.724	1.00 44.36	В
ATOM	2497	CB	GLU E		34.284	35.658	-1.307	1.00 45.65	В
ATOM	2498	CG	GLU E		34.076	37.166	-1.320	1.00 48.42	В
ATOM	2499	CD	GLU E		34.144	37.761	-2.717	1.00 50.71	В
MOTA	2500		GLU E	3 138	35.120	37.471	-3.442	1.00 51.60	В
ATOM	2501		GLU E	3 138	33.227	38.526	-3.086	1.00 50.99	В
MOTA	2502	С	GLU E		33.498	33.335	-1.740	1.00 43.68	В
MOTA	2503	0	GLU I		33.831	32.769	-0.697	1.00 43.53	В
ATOM	2504	N	THR E		33.468	32.711	-2.914	1.00 42.58 1.00 41.76	B B
MOTA	2505	CA	THR I		33.881	31.313	-3.044	1.00 41.76	В
ATOM	2506 2507	CB	THR I		32.739 32.207	30.415 30.948	-3.543 -4.759	1.00 40.71	В
ATOM ATOM	2507		THR		31.641	30.325	-2.492	1.00 41.89	В
ATOM	2509	C	THR I		35.038	31.245	-4.026	1.00 40.93	В
MOTA	2510	ō		B 139	35.855	30.326	-3.981	1.00 40.04	В
MOTA	2511	N		В 140	35.096	32.224	-4.920	1.00 40.67	В

36.179 32.305 -5.887 1.00 41.22 MOTA 2512 CA ALA B 140 В MOTA 2513 CB ALA B 140 35.714 33.016 -7.158 1.00 41.13 В -5.177 ATOM 2514 C ALA B 140 37.247 33.126 1.00 41.09 -4.693 1.00 43.11 В MOTA ALA B 140 36.976 34.232 2515 0 38.455 32.582 -5.102 1.00 39.60 ATOM 2516 N **GLY B 141** В ATOM 2517 CA **GLY B 141** 39.526 33.278 -4.418 1.00 35.11 2518 C **GLY B 141** 39.739 32.651 -3.051 1.00 33.42 ATOM -2.287 ATOM GLY B 141 40.605 33.076 1.00 31.24 2519 O 38.945 1.00 31.89 -2.750 В MOTA 2520 N VAL B 142 31.628 ATOM 2521 CA **VAL B 142** 39.033 30.937 -1.470 1.00 32.27 В -0.813 MOTA VAL B 142 37.645 30.790 1.00 31.90 2522 CB 0.400 1.00 32.37 В CG1 VAL B 142 37.733 29.861 ATOM 2523 ATOM 2524 CG2 VAL B 142 37.125 32.161 -0.402 1.00 32.53 В VAL B 142 39.652 29.552 -1.564 1.00 31.26 В MOTA 2525 C ATOM 2526 O VAL B 142 39.211 28.712 -2.343 1.00 32.44 В 40.676 29.326 -0.752 1.00 30.76 **VAL B 143** В MOTA 2527 N VAL B 143 41.357 28.045 -0.702 1.00 29.79 В MOTA 2528 CA 42.815 28.154 -1.162 1.00 29.63 В ATOM 2529 CB VAL B 143 2530 CG1 VAL B 143 43.439 26.768 -1.212 1.00 31.60 ATOM CG2 VAL B 143 42.885 28.819 -2.514 1.00 33.43 В ATOM 2531 VAL B 143 41.357 27.575 0.749 1.00 30.61 B MOTA 2532 C 1.667 1.00 28.64 MOTA 2533 0 VAL B 143 41.665 28.338 В 41.017 0.950 1.00 29.65 В **SER B 144** 26.313 ATOM 2534 N 40.970 25.756 2.282 1.00 28.42 В ATOM 2535 CA SER B 144 SER B 144 39.541 25.325 2.605 1.00 29.23 В MOTA 2536 CB 1.00 33.81 В OG SER B 144 39.457 24.705 3.875 ATOM 2537 **SER B 144** 41.900 24.562 2.373 1.00 27.32 ATOM 2538 C 1.00 27.40 В 42.101 23.840 1.397 MOTA 2539 **SER B 144** 0 THR B 145 42.492 24.372 3.542 1.00 25.70 В ATOM 2540 N 3.755 1.00 24.82 CA THR B 145 43.364 23.227 В ATOM 2541 44.272 23.418 4.995 1.00 25.01 В THR B 145 ATOM 2542 CB 6.186 43.467 1.00 25.18 В MOTA 2543 OG1 THR B 145 23.399 45.022 24.743 4.923 1.00 23.27 В MOTA 2544 CG2 THR B 145 THR B 145 42.392 22.100 4.071 1.00 24.16 В MOTA C 2545 22.335 4.272 1.00 23.86 41,200 THR B 145 MOTA 2546 0 42.865 4.081 1.00 23.17 В MOTA 2547 N PRO B 146 20.854 MOTA 2548 CD PRO B 146 44.116 20.231 3.618 1.00 22.29 B 1.00 23.18 В PRO B 146 41.854 19.852 4.419 ATOM 2549 CA 18.536 4.008 1.00 24.20 В 42.521 MOTA PRO B 146 2550 CB 4.162 1.00 22.82 В MOTA 2551 CG PRO B 146 43.998 18.833 PRO B 146 41.597 19.945 5.933 1.00 22.63 В MOTA 2552 С 42.213 20.766 6.625 1.00 21.32 В PRO B 146 ATOM 2553 0 40.667 19.146 6.445 1.00 22.60 LEU B 147 MOTA 2554 N 40.414 1.00 22.34 В 7.883 ATOM 2555 CA LEU B 147 19.142 1.00 22.17 **LEU B 147** 39.241 18.216 B.213 В ATOM 2556 CB 38.934 17.973 9.691 1.00 24.53 В CG LEU B 147 ATOM 2557 38.629 19.288 10.368 1.00 25.95 В ATOM 2558 CD1 LEU B 147 1.00 25.55 37.746 17.026 9.826 В ATOM 2559 CD2 LEU B 147 C LEU B 147 41.710 18.609 8.515 1.00 21.99 В ATOM 2560 42.290 17.640 8.024 1.00 21.35 В ATOM LEU B 147 2561 0 42.175 19.246 9.581 1.00 20.48 В TLE B 148 ATOM 2562 N 43.406 18.813 10.228 1.00 19.15 В MOTA 2563 CA ILE B 148 1.00 21.68 ILE B 148 44.392 19.990 10.403 В ATOM 2564 CB 45.666 19.505 11.065 1.00 20.10 В MOTA CG2 ILE B 148 2565 1.00 25.04 CG1 ILE B 148 44.728 20.609 9.041 В MOTA 2566 45.416 1.00 29.06 8.090 В MOTA 2567 CD1 ILE B 148 19.649 1.00 17.56 ILE B 148 43.160 18.208 11.603 В ATOM 2568 С ٥ ILE B 148 42.566 18.852 12.467 1.00 14.88 В MOTA 2569 ARG B 149 43.625 16.973 11.795 1.00 15.95 ATOM 2570 N 1.00 17.47 В CA ARG B 149 43.492 16.273 13.077 2571 ATOM 1.00 16.94 ATOM 2572 CB ARG B 149 43.420 14.763 12.852 В ARG B 149 43.202 13.941 14.128 1.00 20.29 R 2573 CG ATOM ARG B 149 1.00 21.64 43.252 12.448 13.821 В MOTA 2574 CD 1.00 21.97 ARG B 149 42.168 12.028 12.938 MOTA 2575 NB 13.348 1.00 23.22 MOTA 2576 CZ ARG B 149 40.934 11.742 В 40.015 12.471 1.00 23.89 В NH1 ARG B 149 11.374 MOTA 2577 NH2 ARG B 149 40.623 11.803 14.636 1.00 23.11 MOTA 2578 44.720 1.00 17.66 ARG B 149 13.937 16.603 ATOM 2579 C 1.00 17.51 ARG B 149 45.850 16.311 13.549 MOTA 2580 0 ASN B 150 44.496 15.098 1.00 16.67 В 17.210 ATOM 2581 N 1.00 16.94 В ASN B 150 45.592 17.593 15.980 ATOM 2582 CA ASN B 150 16.890 1.00 15.38 ATOM 2583 CB 45.174 18.756 1.00 18.41 CG ASN B 150 16.118 44.899 20.034 ATOM 2584 15.249 1.00 19.05 ATOM 2585 OD1 ASN B 150 45.685 20.436

ATOM	2586	ND2	ASN	В	150	43.790	20.691	16.440	1.00	17.88	В
MOTA	2587	C	ASN	R	150	46.116	16.452	16.841	1 00	18.47	В
ATOM											
	2588	0	asn			47.220	16.540	17.384	1.00	17.03	В
MOTA	2589	И	GLY	В	151	45.324	15.391	16.968	1.00	17.77	В
ATOM	2590	CA	GLY	в	151	45.734	14.251	17.770	1.00	19.16	В
MOTA	2591	C	GLY					19.213			
						45.258	14.293			20.44	В
ATOM	2592	0	GLY	В	151	45.198	13.264	19.877	1.00	22.31	В
ATOM	2593	N	ASP	В	152	44.906	15.475	19.701	1.00	20.79	В
MOTA			ASP								
	2594	CA				44.450	15.624	21.077		21.97	В
MOTA	2595	CB	ASP	В	152	45.192	16.790	21.748	1.00	21.95	В
MOTA	2596	CG	ASP	В	152	45.027	18.101	20.992	1.00	28.05	В
ATOM			ASP			45.764					
	2597						19.060	21.300		30.94	В
MOTA	2598	QD2	ASP	В	152	44.158	18.181	20.090	1.00	28.02	В
ATOM	2599	С	ASP	В	152	42.939	15.847	21.175	1.00	20.51	В
			ASP								
ATOM	2600	0				42.474	16.619	22.010		21.63	В
MOTA	2601	N	TRP	В	153	42.183	15.166	20.322	1.00	19.19	В
ATOM	2602	CA	TRP	в	153	40.724	15.278	20.300	1.00	16.82	В
	.2603	СВ	TRP			40.121					
							14.865	21.657		15.80	В
ATOM	2604	CG	TRP	В	153	40.326	13.408	22.005	1.00	16.21	В
ATOM	2605	CD2	TRP	В	153	39.415	12.322	21.756	1.00	16.58	В
ATOM	2606		TRP			40.047	11.134	22.188		15.08	В
MOTA	2607	CE3	TRP	В	153	38.125	12.238	21.211	1.00	15.69	В
MOTA	2608	CD1	TRP	В	153	41.435	12.848	22.564	1.00	14.68	В
MOTA	2609	MET	TRP	ъ	152	41.278	11.483	22.677	7 00	15.53	В
ATOM	2610	CZ2	TRP			39.438	9.879	22.087	1.00	15.60	В
MOTA	2611	CZ3	TRP	В	153	37.518	10.987	21.112	1.00	14.22	В
ATOM	2612	CH2	TRP	ъ	152	38.176	9.827	21.549		13.89	В
ATOM	2613	С	TRP	В	153	40.194	16.660	19.890	1.00	16.09	В
MOTA	2614	0	TRP	В	153	39.159	17.110	20.379	1.00	14.28	В
ATOM	2615	N	THR	B	154	40.929	17.342	19.020	1 00	15.11	В
ATOM	2616	CA	THR			40.499	18.627	18.483		16.19	В
ATOM	2617	CB	THR	В	154	41.176	19.877	19.150	1.00	18.02	В
ATOM	2618	OG1	THR	В	154	42.602	19.804	19.008	1.00	19.50	В
MOTA		CG2								15.03	В
	2619					40.788	20.000	20.608			
ATOM	2620	C	THR	В	154	40.908	18.602	17.024	1.00	15.24	В
ATOM	2621	0	THR	В	154	41.773	17.832	16.635	1.00	15.24	В
ATOM	2622	N	PHE			40.269	19.437	16.220		18.04	В
MOTA	2623	CA	PHB			40.577	19.538	14.801	1.00	16.03	В
ATOM	2624	CB	PHE	В	155	39.404	19.042	13.938	1.00	16.98	В
ATOM	2625	CG	PHE	R	155	39.069	17.579	14.118	1.00	17.58	В
ATOM	2626		PHE			38.133	17.170	15.074		18.20	В
ATOM	2627	CD2	PHE	В	155	39.670	16.611	13.312	1.00	17.71	В
MOTA	2628	CEI	PHE	R	155	37.799	15.810	15.223	1.00	17.81	В
MOTA	2629		PHB			39.346	15.250	13.451		17.57	В
MOTA	2630	\mathbf{cz}	PHE	В	155	38.407	14.849	14.409	1.00	16.39	В
MOTA	2631	C	PHE	В	155	40.793	21.015	14.503	1.00	16.67	В
	2632		PHE							16.84	В
ATOM		0				40.532	21.870	15.352			
ATOM	2633	N	GLN	В	156	41.281	21.312	13.304	1.00	14.72	В
ATOM	2634	CA	GLN	В	156	41.467	22.689	12.886	1.00	14.66	В
ATOM	2635	CB	GLN			42.811	23.264	13.357	1 00	16.69	В
MOTA	2636	CG	GLN			44.039	22.698	12.669		15.65	В
ATOM	2637	CD	GLN	В	156	45.292	23.486	13.011	1.00	17.87	В
ATOM	2638	OR1	GLN	В	156 .	45.477	24.617	12.555	1.00	17.56	В
			GLN								
MOTA	2639					46.153	22.897	13.830		15.40	В
ATOM	2640	C	GTN	В	156	41.398	22.722	11.371	1.00	14.00	В
ATOM	2641	0	GLN	В	156	41.477	21.691	10.716	1.00	15.17	В
			ILE			41.241	23.911	10.818		15.34	В
ATOM	2642	N									
MOTA	2643	ÇA	IFR	В	157	41.165	24.057	9.383	1.00	17.26	В
ATOM	2644	CB	ILE	В	157	39.791	23.585	8.856	1.00	16.56	В
ATOM	2645		ILE	n	157	38.675	24.429	9.474	1 00	13.07	В
MOTA	2646		ILE			39.765	23.649	7.326		17.72	В
ATOM	2647	CD1	ILE	В	157	38.583	22.913	6.712	1.00	14.50	В
ATOM	2648	C	ILE	В	157	41.379	25.523	9.074	1.00	18.67	В
MOTA	2649	0			157	40.823	26.391	9.745		22.28	В
MOTA	2650	N	LEU	В	158	42.217	25.795	8.083	1.00	18.98	В
MOTA	2651	CA	LEU	В	158	42.508	27.162	7.690	1.00	20.77	В
			LEU					7.555		22.23	
MOTA	2652	CB				44.022	27.368				В
ATOM	2653	CG			158	44.851	27.525	8.838		26.12	В
ATOM	2654	CD1	LEU	В	158	44.689	26.320	9.740	1.00	29.01	В
ATOM	2655		LEU			46.311	27.701	8.465		28.46	В
MOTA	2656	C			158	41.817	27.484	6.371		20.61	В
ATOM	2657	0	LEU	В	158	41.934	26.734	5.401	1.00	19.39	В
ATOM	2658	N			159	41.088	28.596	6.346	1.00	21.67	В
MOTA	2659	CA	AMP	ಶ	159	40.380	29.011	5.141	1.00	21.90	В

MOTA	2660	СВ	VAL B	159	38.855	29.061	5.365	1.00 22.06	В
MOTA	2661		VAL B		38.147	29.252	4.043	1.00 20.55	В
MOTA	2662		VAL B		38.381	27.766	6.009	1.00 20.83	В
ATOM ATOM	2663 2664	C 0	VAL B		40.899 40.721	30.379 31.357	4.749 5.473	1.00 21.80 1.00 20.82	B
ATOM	2665	N	MET B		41.555	30.416	3.592	1.00 23.56	В
ATOM	2666	CA	MET B		42.179	31.613	3.055	1.00 25.12	В
MOTA	2667	CB	MET B	160	43.580	31.257	2.559	1.00 26.80	В
MOTA	2668	CG	MET B		44.479	30.736	3.678	1.00 32.00	В
MOTA	2669	SD	MET B		45.850	29.700	3.145	1.00 38.02	В
ATOM ATOM	2670 2671	CE CE	MET B		45.094 41.387	28.065 32.269	3.307 1.941	1.00 35.43 1.00 28.27	B
ATOM	2672	ŏ	MET B		40.684	31.602	1.177	1.00 28.76	В
ATOM	2673	N	LEU B		41.518	33.588	1.854	1.00 29.59	В
MOTA	2674	CA	LEU B		40.820	34.366	0.845	1.00 32.69	В
MOTA	2675	СВ	PEG B		39.669	35.142	1.487	1.00 30.80	В
ATOM	2676	CG	LEU B		39.031 38.156	36.199 35.516	0.586 -0.460	1.00 31.56 1.00 29.64	B B
MOTA	2677 2678		LEU B		38.213	37.167	1.423	1.00 29.89	В
ATOM	2679	c	LEU B		41.755	35.349	0.154	1.00 35.59	В
ATOM	2680	0	LEU B	161	42.350	36.216	0.801	1.00 35.54	В
ATOM	2681	N	GLU B		41.895	35.203	-1.158	1.00 39.87	В
ATOM	2682	CA	GLU B		42.728	36.118	-1.927	1.00 44.05	В
MOTA	2683 2684	CB CG	GLU B		42.995 43.795	35.565 36.497	-3.331 -4.239	1.00 46.86 1.00 50.98	B
ATOM ATOM	2685	CD	GLU B		45.274	36.537	-3.891	1.00 54.75	В
ATOM	2686		GLU B		45.604	36.802	-2.715	1.00 56.53	В
ATOM	2687		GLU B		46.108	36.308	-4.796	1.00 55.16	В
MOTA	2688	C	GLU B		41.879	37.372	-2.029	1.00 44.69	В
MOTA	2689	0	GLU B		40.719	37.302	-2.434	1.00 44.39	В
ATOM ATOM	2690 2691	N CA	MET B		42.436 41.670	38.514 39.746	-1.648 -1.716	1.00 46.67 1.00 49.56	B B
ATOM	2692	CB	MET B		40.881	39.949	-0.412	1.00 51.22	В
MOTA	2693	CG	MET B		41.652	39.675	0.876	1.00 51.58	В
ATOM	2694	SD	MET B	163	42.910	40.901	1.274	1.00 56.87	В
MOTA	2695	CE		163	41.915	42.187	2.029	1.00 54.89	В
ATOM	2696	C	MET B	163	42.487 43.717	40.986 40.988	-2.028 -1.942	1.00 51.43 1.00 51.02	B B
ATOM ATOM	2697 2698	N	THR B		43.717	42.038	-2.412	1.00 51.02	В
ATOM	2699	CA	THR B		42.385	43.316	-2.738	1.00 56.61	В
ATOM	2700	CB	THR B	164	41.889	43.820	-4.116	1.00 57.48	В
MOTA	2701	OG1			40.457	43.744	-4.172	1.00 57.81	В
MOTA	2702	CG2			42.480	42.967	-5.234	1.00 57.23 1.00 57.80	B B
ATOM ATOM	2703 2704	0	THR B		42.012 40.866	44.318 44.766	-1.642 -1.555	1.00 57.08	В
ATOM	2705	N	PRO B		42.976	44.658	-0.770	1.00 58.98	В
ATOM	2706	CD	PRO E	165	44.315	44.055	-0.647	1.00 59.54	В
MOTA	2707	CA	PRO P		42.734	45.605	0.322	1.00 60.52	В
MOTA	2708	СВ	PRO E		44.063	45.608	1.078	1.00 60.33 1.00 60.42	В
MOTA MOTA	2709 2710	CG C	PRO P		44.604	44.236 47.002	0.822 -0.163	1.00 60.42	B B
ATOM	2711	0	PRO E		43.149	47.698	-0.790	1.00 61.24	В
ATOM	2712	N	GLN E		41.110	47.395	0.126	1.00 62.45	В
ATOM	2713	CA	GLN E		40.598	48.709	-0.250	1.00 63.32	В
ATOM	2714	CB	GLN E		39.605	48.590	-1.410	1.00 65.46	В
MOTA	2715	CG	GLN E		40.177	47.945 47.942	-2.661 -3.819	1.00 69.00 1.00 71.19	B
ATOM ATOM	2716 2717	CD OE1	GILN I		38.071	47.448	-3.697	1.00 72.48	В
ATOM	2718	NE2			39.617	48.492	-4.954	1.00 72.65	В
ATOM	2719	C	GLN I		39.893	49.287	0.970	1.00 62.65	В
MOTA	2720	0	GLN I		39.021	48.635	1.550	1.00 62.16	. в
MOTA	2721	N	ARG I		40.266	50.501	1.366	1.00 61.62 1.00 60.86	B
MOTA MOTA	2722 2723	CA CB	ARG I		39.645 40.190	51.111 52.525	2.535 2.777	1.00 60.86	В
ATOM	2724	CG	ARG I		39.953	53.029	4.204	1.00 64.82	В
ATOM	2725	Œ	ARG I	3 167	40.742	52.198	5.227	1.00 67.31	В
MOTA	2726	NE		B' 167	40.094	52.143	6.539	1.00 69.03	В
ATOM	2727	CZ		B 167	40.570	51.477	7.591	1.00 69.14	В
MOTA	2728 2729		ARG I		41.710 39.897	50.804 51.471	7.499 8.735	1.00 69.34 1.00 69.52	B
MOTA MOTA	2730	C		B 167	38.136	51.154	2.333	1.00 59.19	В
MOTA	2731	ō		B 167	37.647	51.615	1.303	1.00 58.60	В
ATOM	2732	N		B 168	37.404	50.656	3.320	1.00 58.18	В
MOTA	2733	CA	GLY :	B 168	35.959	50.632	3.226	1.00 56.57	В

MOTA	2734	С	GLY B	168	35.466	49.200	3.191	1.00 55.42	В
ATOM	2735	0	GLY B	168	34.306	48.924	3.495	1.00 55.98	В
MOTA	2736	N	ASP B	169	36.350	48.280	2.814	1.00 53.44	В
ATOM	2737	CA	ASP B	169	35.979	46.871	2.757	1.00 51.76	В
ATOM	2738	CB	ASP B		36.841	46.115	1.740	1.00 50.49	В
ATOM	2739	CG	ASP B		36.428	46.392	0.311	1.00 50.57	В
ATOM	2740		ASP B		35.207	46.479	0.060	1.00 49.92	В
ATOM	2741	OD2	ASP B	169	37.31B	46.507	-0.559	1.00 49.84	В
MOTA	2742	C	ASP B		36.083	46.181	4.110	1.00 49.36	В
ATOM	2743	0	ASP B		37.066	46.343	4.836	1.00 48.92	В
MOTA	2744	N	VAL B		35.047	45.418	4.436	1.00 47.48	В
ATOM	2745	CA	VAL B		34.981	44.667	5.680	1.00 45.10	В
ATOM	2746	CB	VAL B		33.800	45.130	6.543	1.00 45.86	В
MOTA	2747		VAL B		33.702	44.268	7.795	1.00 46.26	В
MOTA	2748		VAL B		33.974	46.598	6.906	1.00 46.23	В
ATOM	2749	C	VAL B		34.787	43.191	5.342	1.00 43.62	В
ATOM	2750	0	VAL B		33.774	42.807	4.762	1.00 42.86	В
ATOM	2751	N	TYR B		35.762	42.367	5.704	1.00 41.69	В
MOTA	2752	CA	TYR B		35.694	40.935	5.425	1.00 38.95	В
MOTA	2753	СВ	TYR B		37.044	40.455	4.899	1.00 37.52	В
ATOM	2754	CG	TYR B		37.405	41.031	3.553	1.00 38.12	В
ATOM	2755		TYR B		37.023	40.391	2.376	1.00 37.52	В
ATOM	2756		TYR B		37.342	40.923	1.131	1.00 38.06	В
ATOM	2757		TYR B		38.118	42.224	3.454	1.00 37.54	В
ATOM	2758	CE2	TYR B		38.442 38.052	42.767	2.216	1.00 38.45	B B
MOTA	2759	CZ OH	TYR B			42.110 42.641	1.056 -0.172	1.00 39.25	В
MOTA	2760	C	TYR B		38.372 35.314	40.139	6.671	1.00 37.46	В
MOTA MOTA	2761 2762	0	TYR B		35.791	40.428	7.773	1.00 34.85	В
ATOM	2763	N	THR B		34.452	39.140	6.501	1.00 35.06	В
ATOM	2764	CA	THR B		34.049	38.328	7.638	1.00 35.81	В
ATOM	2765	CB	THR B		32.589	38.622	8.064	1.00 38.37	В
ATOM	2766		THR B		31.688	38.177	7.043	1.00 42.02	В
MOTA	2767	CG2	THR B		32.390	40.119	8.292	1.00 39.83	В
ATOM	2768	C	THR B		34.182	36.830	7.406	1.00 33.71	В
MOTA	2769	0	THR B		33.953	36.335	6.300	1.00 32.99	В
ATOM	2770	N	CYS B		34.578	36.123	8.463	1.00 32.09	В
ATOM	2771	CA	CYS B	173	34.714	34.670	8.438	1.00 31.08	В
MOTA	2772	C	CYS B	173	33.497	34.183	9.200	1.00 30.92	В
MOTA	2773	0	CYS B	173	33.240	34.614	10.326	1.00 32.70	В
MOTA	2774	CB	CYS B	173	35.988	34.214	9.155	1.00 31.48	В
MOTA	2775	SG	CYS B		36.338	32.436	8.983	1.00 31.85	В
MOTA	2776	N	HIS B		32.748	33.288	8.578	1.00 30.26	В
MOTA	2777	CA	HIS B		31.524	32.754	9.152	1.00 29.72	В
MOTA	2778	СВ	HIS B		30.401	32.977	8.128	1.00 30.80	В
ATOM	2779	CG	HIS B		29.030	32.625	8.615	1.00 32.90	В
MOTA	2780		HIS E		28.016	33.405	9.058	1.00 33.11	В
ATOM	2781		HIS E		28.551	31.332	8.621	1.00 34.85	В
ATOM	2782		HIS E		27.299	31.332	9.044	1.00 37.21	B B
MOTA	2783		HIS E		26.950	32.577 31.271	9.316 9.449	1.00 34.95 1.00 28.49	В
ATOM	2784	0	HIS E		31.751	30.494	8.554	1.00 27.69	В
ATOM	2785	-	VAL E		32.080 31.584	30.888	10.710	1.00 27.48	В
ATOM	2786 2787	n Ca	VAL E		31.810	29.508	11.121	1.00 25.94	В
MOTA	2788	СВ	VAL E		32.988	29.418	12.126	1.00 25.31	В
MOTA	2789		VAL E		33.147	27.982	12.629	1.00 21.10	В
MOTA	2790		VAL		34.271	29.896	11.462	1.00 22.12	В
MOTA	2791	C	VAL E		30.606	28.821	11.748	1.00 26.58	В
MOTA	2792	ō	VAL E		30.004	29.328	12.694	1.00 27.01	В
MOTA	2793	N	GLU E		30.274	27.652	11.212	1.00 27.17	В
ATOM	2794	CA	GLU E		29.168	26.846	11.712	1.00 28.51	В
MOTA	2795	СВ	GLU I		28.166	26.573	10.588	1.00 32.35	В
ATOM	2796	CG	GLU I		27.454	27.827	10.082	1.00 38.87	В
MOTA	2797	æ	GLU F	3 176	26.776	27.616	8.735	1.00 42.45	В
MOTA	2798		GLU I		25.947	26.684	8.618	1.00 43.07	В
MOTA	2799	OE2	GLU I	B 176	27.075	28.386	7.794	1.00 42.94	В
ATOM	2800	C	GLU I	B 176	29.750	25.536	12.235	1.00 27.34	В
ATOM	2801	0	GLU I	B 176	30.576	24.900	11.574	1.00 26.12	В
ATOM	2802	N		B 177	29.308	25.134	13.420	1.00 26.08	В
ATOM	2803	CA		B 177	29.800	23.921	14.049	1.00 26.30	В
ATOM	2804	CB		B 177	31.132	24.244	14.738	1.00 24.58	В
MOTA	2805	CG		B 177	31.759	23.076	15.422	1.00 22.32	В
MOTA	2806		HIS		32.646	22.156	14.977	1.00 21.05	В
MOTA	2807	ND	HIS	B 177	31.437	22.711	16.710	1.00 21.01	В

				22 007	21 612	17 020	1.00 23.72	В
ATOM	2808		HIS B 177	32.097	21.613	17.030		
MOTA	2809	NE2	HIS B 177	32.838	21.255	15.995	1.00 23.87	В
MOTA	2810	C	HIS B 177	28.762	23.413	15.057	1.00 27.87	В
ATOM	2811	0	HIS B 177	28.059	24.205	15.672	1.00 29.54	В
MOTA	2812	N	PRO B 178	28.654	22.085	15.237	1.00 29.57	В
ATOM	2813	CD	PRO B 178	29.365	21.025	14.501	1.00 28.96	В
		CA	PRO B 178	27.687	21.497	16.175	1.00 31.71	В
ATOM	2814				20.019	16.166	1.00 30.49	В
MOTA	2815	CB	PRO B 178	28.062				
MOTA	2816	CG	PRO B 178	28.503	19.810	14.769	1.00 30.01	В
ATOM	2817	C	PRO B 178	27.649	22.071	17.595	1.00 33.29	В
ATOM	2818	0	PRO B 178	26.619	22.020	18.256	1.00 35.00	В
MOTA	2819	N	SER B 179	28.762	22.615	18.067	1.00 34.96	В
		CA	SER B 179	28.813	23.168	19.418	1.00 36.85	В
MOTA	2820					19.896	1.00 35.35	В
ATOM	2821	CB	SER B 179	30.261	23.228			
ATOM	2822	OG	SER B 179	31.023	24.053	19.034	1.00 35.14	В
MOTA	2823	C	SER B 179	28.206	24.564	19.522	1.00 38.40	В
ATOM	2824	0	SER B 179	27.953	25.056	20.619	1.00 37.27	В
ATOM	2825	N	LEU B 180	27.971	25.192	18.377	1.00 40.10	В
		CA	LEU B 180	27.434	26.545	18.340	1.00 41.36	В
ATOM	2826					17.269	1.00 39.74	В
MOTA	2827	CB	LEU B 180	28.162	27.352			В
MOTA	2828	CG	LEU B 180	29.677	27.432	17.422	1.00 39.93	
ATOM	2829	CD1	LEU B 180	30.286	28.013	16.157	1.00 39.41	В
MOTA	2830	CD2	LEU B 180	30.021	28.279	18.636	1.00 39.61	В
ATOM	2831	C	LEU B 180	25.944	26.633	18.078	1.00 43.85	В
	2832	ŏ	LEU B 180	25.449	26.125	17.072	1.00 44.25	В
ATOM					27.289	18.984	1.00 47.20	В
MOTA	2833	N	GLN B 181	25.230			1.00 49.93	В
ATOM	2834	CA	GLN B 181	23.794	27.475	18.814		
MOTA	2835	CB	GLN B 181	23.158	27.956	20.121	1.00 52.00	B
ATOM	2836	CG	GLN B 181	23.873	29.134	20.758	1.00 56.40	В
MOTA	2837	CD	GLN B 181	23.263	29.538	22.084	1.00 59.03	В
ATOM	2838		GLN B 181	22.087	29.908	22.153	1.00 60.55	В
		NE2		24.059	29.468	23.149	1.00 58.44	В
MOTA	2839				28.522	17.715	1.00 49.23	В
MOTA	2840	С	GLN B 181	23.635				В
MOTA	2841	0	GLN B 181	22.712	28.465	16.906	1.00 49.91	
ATOM	2842	N	SER B 182	24.560	29.474	17.688	1.00 48.48	В
ATOM	2843	CA	SER B 182	24.555	30.523	16.679	1.00 47.89	В
MOTA	2844	CB	SER B 182	24.241	31.879	17.314	1.00 48.68	В
ATOM	2845	OG	SER B 182	25.211	32.223	18.286	1.00 50.58	В
ATOM	2846	c	SER B 182	25.938	30.550	16.038	1.00 45.93	В
				26.945	30.354	16.714	1.00 45.13	В
MOTA	2847	0	SER B 182			14.721	1.00 45.12	В
ATOM	2848	N	PRO B 183	26.004	30.783			
ATOM	2849	CD	PRO B 183	24.911	31.096	13.784	1.00 44.93	B
ATOM	2850	CA	PRO B 183	27.302	30.819	14.042	1.00 43.29	В
MOTA	2851	СВ	PRO B 183	26.923	31.070	12.581	1.00 43.70	В
ATOM	2852	CG	PRO B 183	25.642	31.833	12.688	1.00 44.70	В
ATOM	2853	c	PRO B 183	28.254	31.876	14.593	1.00 40.67	В
				27.828	32.851	15.209	1.00 40.46	В
MOTA	2854	0	PRO B 183			14.382	1.00 37.76	В
MOTA	2855	N	ILE B 184	29.547				
MOTA	2856	CA	ILE B 184	30.550	32.607	14.842	1.00 35.88	В
MOTA	2857	CB	ILE B 184	31.759	31.889	15.468	1.00 35.92	В
ATOM	2858	CG	2 ILE B 184	32.907	32.867	15.657	1.00 35.57	В
ATOM	2859	CG	1 ILE B 184	31.362	31.270	16.806	1.00 36.74	В
MOTA	2860		1 ILE B 184		30.477	17.458	1.00 36.59	В
			ILE B 184			13.680	1.00 34.88	В
MOTA	2861	C				12.630	1.00 35.06	В
MOTA	2862	0	ILE B 184	_				В
MOTA	2863	N	THR B 185			13.876	1.00 34.50	
MOTA	2864	ÇA	THR B 185	31.500	35.675	12.845	1.00 34.32	В
MOTA	2865	CB	THR B 185	30.356	36.592	12.341	1.00 35.40	В
ATOM	2866		1 THR B 185	29.770	37.285	13.450	1.00 37.01	В
MOTA	2867		2 THR B 185			11.631	1.00 35.73	В
			THR B 185			13.375		В
MOTA	2868					14.494		В
MOTA	2869		THR B 185			12.560		В
MOTA	2870		VAL B 186					
ATOM	2871	. CA						В
MOTA	2872	CE	VAL B 186	36.041		13.155		В
ATOM	2873	CG	1 VAL B 186	37.212	37.570			В
ATOM	2874		2 VAL B 186			14.262	1.00 33.67	В
ATOM	2875		VAL B 186				1.00 34.68	В
	2876		VAL B 186					В
MOTA								В
ATOM	2877		GLU B 187					В
MOTA	2878							
MOTA	2879							В
MOTA	2880) CC	GLU B 18'	7 33.008				В
ATOM	2881	L CI	GLU B 18	7 32.146	5 42.876	11.421	1.00 48.81	В

ATOM	2882		GLU B		30.909	42.739	11.545	1.00 51.77	В
ATOM ATOM	2883 2884	OE2	GLU B		32.701 36.816	43.997 41.175	11.363 10.784	1.00 49.79 1.00 39.59	B B
ATOM	2885	0	GLU B		37.637	40.998	11.684	1.00 39.84	В
ATOM	2886	N	TRP B	188	37.113	41.765	9.635	1.00 39.59	В
ATOM	2887	CA	TRP B		38.430	42.302	9.360	1.00 40.86	В
ATOM	2888	СВ	TRP B		39.339	41.252 41.704	8.736	1.00 38.70 1.00 37.82	B B
ATOM	2889 2890	CG	TRP B		40.769 41.421	42.383	8.693 7.615	1.00 37.62	В
ATOM ATOM	2891		TRP B		42.748	42.640	8.023	1.00 36.31	В
ATOM	2892	CE3	TRP B		41.013	42.799	6.340	1.00 36.14	В
ATOM	2893	CD1	TRP B	188	41.698	41.583	9.686	1.00 37.31	В
ATOM	2894	NE1			42.890	42.141	9.291	1.00 37.27	B
MOTA	2895	CZ2	TRP B		43.673 41.932	43.296 43.452	7.204 5.522	1.00 37.17 1.00 38.70	В
ATOM ATOM	2896 2897	CZ3 CH2	TRP B		43.249	43.694	5.960	1.00 37.13	В
ATOM	2898	C	TRP B		38.258	43.455	8.383	1.00 42.97	В
MOTA	2899	0	TRP B		37.946	43.240	7.211	1.00 42.37	В
ATOM	2900	N	ARG B		38.442	44.678	8.864	1.00 46.69 1.00 50.32	B B
ATOM	2901	CA CB	ARG B		38.303 37.731	45.842 47.040	7.999 8.776	1.00 50.32	В
MOTA MOTA	2902 2903	CG	ARG B		38.615	47.590	9.893	1.00 56.00	В
ATOM	2904	CD	ARG B		38.234	47.041	11.270	1.00 59.95	В
ATOM	2905	NE	ARG B		38.639	45.650	11.479	1.00 63.62	В
ATOM	2906	CZ	ARG B		39.903	45.236	11.559	1.00 64.33 1.00 65.45	B B
ATOM	2907		ARG B		40.899 40.172	46.105 43.951	11.447 11.760	1.00 65.45	В
ATOM ATOM	2908 2909	NH2	ARG E		39.664	46.192	7.412	1.00 50.56	В
ATOM	2910	ŏ	ARG E		40.680	46.119	8.100	1.00 50.34	В
MOTA	2911	N	ALA E	190	39.684	46.554	6.135	1.00 52.30	В
ATOM	2912	CA	ALA E		40.933	46.911	5.476	1.00 54.16 1.00 55.33	B B
ATOM	2913	СВ	ALA E		40.846 41.238	46.592 48.392	3.987 5.679	1.00 55.33	В
MOTA MOTA	2914 2915	C	ALA E		40.300	49.147	6.023	1.00 54.90	В
ATOM	2916		ALA E		42.408	48.782	5.481	1.00 56.19	В
MOTA	2917	C	LEU (32.073	1.033	33.225	1.00 35.70	C
ATOM	2918	0	LEU C		33.091	1.607	33.619	1.00 35.87 1.00 36.17	c c
MOTA	2919	N CA	LEU (29.791 30.699	1.906 1.409	32.702 33.777	1.00 34.35	c
MOTA MOTA	2920 2921	N	GIN (32.105	0.072	32.307	1.00 34.64	C
MOTA	2922	CA	GLN (33.374	-0.359	31.737	1.00 34.20	C
ATOM	2923	С	GTW (33.250	-0.823	30.294	1.00 33.55	C
MOTA	2924	0	GIM (32.373 34.130	-1.610 -0.329	29.955 29.418	1.00 33.68 1.00 33.74	ď
ATOM ATOM	2925 2926	N CD	PRO (35.226	0.632	29.639	1.00 33.81	č
ATOM	2927	CA	PRO		34.064	-0.742	28.015	1.00 34.77	C
MOTA	2928	CB	PRO (С 3	35.027	0.222	27.329	1.00 34.33	C
MOTA	2929	CG	PRO		36.070	0.449	28.393	1.00 34.78	C
MOTA	2930	C	PRO		34.508 35.435	-2.195 -2.626	27.890 28.579	1.00 34.42 1.00 34.76	c
MOTA MOTA	2931 2932	O N	PRO (33.837	-2.947	27.024	1.00 31.97	Ċ
MOTA	2933	CA	PHE		34.173	-4.355	26.812	1.00 32.26	C
MOTA	2934	СВ	PHE		32.897	-5.193	26.632	1.00 34.22	c
MOTA	2935	CG			32.006	-5.235	27.852	1.00 37.02	C
MOTA	2936		1 PHE		32.481 30.701	-4.835 -5.726	29.103 27.756	1.00 38.53 1.00 40.29	Č
MOTA MOTA	2937 2938		1 PHE		31.673	-4.925	30.248	1.00 40.80	C
ATOM	2939		2 PHE		29.878	-5.824	28.891	1.00 41.19	C
MOTA	2940	CZ			30.369	-5.421	30.142	1.00 40.74	C
MOTA	2941		PHE		35.052	-4.483 -4.072	25.571 24.482	1.00 29.17 1.00 30.93	C
ATOM	2942 2943		PHE		34.655 36.257		25.715	1.00 26.63	č
MOTA MOTA	2944				36.936			1.00 24.97	C
MOTA	2945				37.168	-5.217		1.00 23.69	C
ATOM	2946	CB	PRO	C 5	38.527				C
MOTA	2947				38.335				C
MOTA	2948		PRO		37.043 36.403				c
MOTA MOTA	2949 2950		GLN		37.666				C
ATOM	2951				37.659	-7.945	21.967	1.00 21.10	C
MOTA	2952				37.506				c
MOTA	2953				36.170				c
MOTA MOTA	2954 2955		GLN		36.074 36.483				č
MIOM	4335	. 08	·* 6mg	- 0	JJ. 703				_

ATOM	2956	MES	GLN	~	6	35.525	-5.766	18.149	1.00 20.70	С
ATOM	2957	C	GLN		6	38.996	-8.637	22.204	1.00 20.71	C
ATOM	2958	0	GLN		6	40.046	-8.008	22.105	1.00 19.85	C
ATOM	2959	N	PRO		7	38.974	-9.932	22.548	1.00 21.37	С
MOTA	2960	CD	PRO	С	7	37.810	-10.710	23.017	1.00 21.21	С
ATOM	2961	CA	PRO	C	7	40.215	-10.673	22.790	1.00 21.62	C
ATOM	2962	CB	PRO	C	7	39.783	-11.730	23.795	1.00 21.96	C
MOTA	2963	CG	PRO	C	7	38.416	-12.085	23.297	1.00 20.65	C
ATOM	2964	C	PRO		7	40.741	-11.316	21.511	1.00 24.05	C
ATOM	2965	ō	PRO		7		-11.577	20.588	1.00 22.84	č
ATOM	2966	N	GLU		8		-11.550	21.448	1.00 26.22	č
										č
ATOM	2967	CA	GLU		8		-12.215	20.292	1.00 27.00	
ATOM	2968	CB	GLU		8		-11.687	19.988	1.00 27.94	c
MOTA	2969	CG	GLU		8		-12.494	18.915	1.00 28.38	C
ATOM	2970	CD	GLU	С	8	44.043	-12.649	17.589	1.00 31.32	C
MOTA	2971	OE1	GLU	C	8	42.980	-13.309	17.564	1.00 31.69	С
MOTA	2972	OE2	ಡಗಿರ	C	8	44.514	-12.112	16.563	1.00 29.86	C
ATOM	2973	C	GLU	С	8	42.678	-13.691	20.676	1.00 28.48	C
ATOM	2974	0	GLU	C	8	42.937	-14.029	21.829	1.00 28.74	C
ATOM	2975	N	LEU		9		-14.571	19.721	1.00 30.08	C
MOTA	2976	CA	LEU		9		-15.998	20.002	1.00 31.21	c
ATOM		CB	LEU		9		-16.688	19.183	1.00 32.12	č
	2977				9				1.00 32.12	c
MOTA	2978	CG.	LEU				-16.072	19.302		
ATOM	2979		LEU		9		-16.866	18.457	1.00 35.00	C
ATOM	2980		LEU		9		-16.061	20.761	1.00 35.59	C
MOTA	2981	С	I'EA	С	9	43.748	-16.641	19.712	1.00 31.83	С
MOTA	2982	0	LEU	C	9	44.342	-16.415	18.658	1.00 30.94	C
MOTA	2983	N	PRO	С	10	44.256	-17.442	20.657	1.00 33.31	C
ATOM	2984	CD	PRO	C	10	43.774	-17.661	22.032	1.00 33.12	C
ATOM	2985	CA	PRO	С	10	45.545	-18.097	20.439	1.00 36.08	C
MOTA	2986	СВ	PRO		10		-18.590	21.836	1.00 36.62	С
ATOM	2987	CG	PRO		10		-18.846	22.476	1.00 35.26	Ċ
	2988	C	PRO		10		-19.229	19.430	1.00 37.51	č
MOTA									1.00 37.31	č
ATOM	2989	0	PRO		10		-20.030	19.491		
ATOM	2990	N	TYR		11		-19.269	18.488	1.00 38.68	c
ATOM	2991	CA	TYR	С	11		-20.305	17.463	1.00 40.24	С
ATOM	2992	C	TYR	С	11	47.834	-20.782	17.290	1.00 42.03	C
MOTA	2993	0	TYR	C	11	48.121	-21.967	17.586	1.00 42.72	C
ATOM	2994	OXT	TYR	C	11	48.665	-19.949	16.870	1.00 42.75	C
ATOM	2995	CB	VAL	D	2	76.722	40.050	4.030	1.00 35.81	D
ATOM	2996		VAL		2	77.537		2.823	1.00 36.64	D
ATOM	2997		VAL		2	76.313	38.577	3.893	1.00 37.71	D
ATOM	2998	C	VAL		2	76.622	40.298		. 1.00 31.61	D
ATOM	2999	Ö	VAL		2	75.696	39.494	6.653	1.00 31.96	D
						78.625		5.418	1.00 32.12	D
MOTA	3000	N	VAL		2				1.00 32.12	D
ATOM	3001	CA	VAL		2	77.560		5.317		
MOTA	3002	N	ALA		3	76.864		7.441	1.00 29.52	D
MOTA	3003	ÇA	ALA		3	76.053		8.653	1.00 27.92	D
ATOM	3004	CB	ALA	D	3	76.480	40.321	9.684	1.00 27.11	D
MOTA	3005	C	ALA	D	3	76.128	42.767	9.286	1.00 25.71	D
ATOM	3006	0	ALA	. D	3	77.050	43.540	9.016	1.00 23.11	D
MOTA	3007	N	ASP	D	4	75.152		10.137	1.00 24.26	D
ATOM	3008	CA	ASP	D	4	75.109	44.354	10.825	1.00 24.77	D
ATOM	3009	CB	ASP		4	73.774		11.555	1.00 25.88	D
ATOM	3010	CG	ASP		4	72.595		10.611	1.00 26.24	D
ATOM	3011		ASP		4	71.449		11.080	1.00 24.74	D
MOTA	3012		ASP		4	72.811		9.416	1.00 28.25	D
ATOM						76.230		11.857	1.00 25.96	D
	3013	C	ASP		4			12.027	1.00 26.40	Ď
MOTA	3014	0	ASP		4	76.882				
ATOM	3015	N	HIS		5	76.440		12.549	1.00 24.52	D
MOTA	3016	CA	HIS		5	77.469		13.582	1.00 24.25	D
ATOM	3017	CB	HIS	D	5	76.836		14.972	1.00 23.42	D
MOTA	3018	CG	HIS	D	5	76.138	44.599	15.231	1.00 26.12	D
MOTA	3019	CD2	HIS	D	5	76.567	45.879	15.126	1.00 26.16	D
MOTA	3020	NDI	. HIS	D	5	74.830	44.667	15.657	1.00 25.67	D
MOTA	3021		HIS		5	74.481		15.799	1.00 26.53	D
MOTA	3022		HIS		5	75.516		15.484	1.00 25.96	D
ATOM	3023	C	HIS		5	78.241		13.492	1.00 22.88	D
ATOM	3024	ō	HIS		5	77.657		13.258	1.00 22.31	D
ATOM	3025	N	VAL		6	79.552		13.691	1.00 20.27	D
ATOM	3025					80.421		13.657	1.00 19.49	D
		CA	VAI		6.			12.486	1.00 19.49	D
ATOM	3027	CB	VAI		6.	81.419			1.00 20.45	D
ATOM	3028		VAI		6	82.357		12.564		D
MOTA	3029	CG2	IAV S	םי	6	80.674	40.869	11.161	1.00 25.29	U

ATOM 3030 C VAL D 81.223 40.792 14.944 1.00 18.77 VAL D MOTA 3031 0 6 81.767 41.812 15.352 1.00 17.70 3032 N ALA D 81.304 39.626 15.575 MOTA 7 1.00 18.23 3033 CA ALA D ATOM 7 82.046 39.489 16.821 1.00 18.01 ATOM 3034 CB ALA D 81.080 39.452 18.006 1.00 17.61 MOTA 3035 C ALA D 82.899 38.239 16.838 1.00 17.37 3036 O ALA D 82.568 MOTA 7 37.242 16.208 1.00 19.56 ATOM 3037 N SER D 8 84.008 38.306 17.562 1.00 17.07 84.892 ATOM 3038 CA SER D 8 37.158 17.712 1.00 15.46 MOTA 3039 СВ SER D 86.297 37.455 17.202 1.00 12.56 8 3040 OG SER D 86,324 ATOM 8 37.492 15.789 1.00 18.97 ATOM 3041 C SER D 8 84.932 36.904 19.201 1.00 16.39 ATOM 3042 0 SER D 8 85.613 37.614 19.951 1.00 15.61 84.144 1.00 17.58 3043 N TYR D 35.930 19.637 ATOM 9 84.096 21.044 1.00 18.51 ATOM 3044 CA TYR D 9 35.587 D 3045 CB TYR D 9 82.698 35.133 21.444 1.00 17.92 ATOM D ATOM CG TYR D 9 81.730 36.290 21.362 1.00 17.41 3046 82.056 CD1 TYR D 37.523 21.928 1.00 16.27 ATOM 3047 9 81.208 MOTA 3048 CE1 TYR D 9 38.603 21.840 1.00 15.18 D ATOM 3049 CD2 TYR D 9 80.515 36.169 20.701 1.00 17.05 D 20.608 1.00 18.01 MOTA 3050 CE2 TYR D 9 79.649 37.252 80.005 38.466 21.181 1.00 16.67 MOTA 3051 CZ TYR D 9 79.157 39.543 21.104 1.00 20.30 MOTA 3052 OH TYR D 9 3053 C TYR D 9 85.120 34.508 21.115 1.00 19.92 D ATOM TYR D 9 84.856 33.323 21.337 1.00 17.21 MOTA 3054 O 86.321 34.989 1.00 22.61 3055 N GLY D 10 20.843 MOTA 20.836 1.00 20.96 MOTA 3056 CA GLY D 10 87.478 34.160 3057 C GLY D 10 88.358 34.354 19.624 1.00 18.79 MOTA 88.170 1.00 16.79 ATOM 3058 O GLY D 10 33.693 18.618 VAL D 11 3059 N 89.275 35.307 19.683 1.00 17.75 MOTA 18.616 1.00 16.92 3060 CA VAL D 11 90,256 35.394 MOTA 3061 CB VAL D 11 90.666 36.829 18.242 1.00 17.76 MOTA 3062 CG1 VAL D 11 91.873 36.778 17.313 1.00 15.46 MOTA 3063 CG2 VAL D 11 89.522 37.544 17.544 1.00 13.00 MOTA 91.391 34.728 19.395 1.00 17.46 VAL D 11 MOTA 3064 C 91.865 35.266 20.405 1.00 18.93 MOTA 3065 O VAL D 11 MOTA 3066 N ASN D 12 91.773 33.531 18.973 1.00 17.46 3067 CA ASN D 12 92.831 32.779 19.644 1.00 18.01 MOTA 3068 CB ASN D 12 92.339 1.00 16.68 31.360 19.969 D MOTA 1.00 16.27 ATOM 3069 CG ASN D 12 91.179 31.356 20.955 D OD1 ASN D 12 91.346 30.989 22.115 1.00 14.97 MOTA 3070 90.000 ND2 ASN D 12 31.779 20.497 1.00 14.97 MOTA 3071 18.759 1.00 18.74 94.061 32.699 MOTA 3072 С ASN D 12 ASN D 12 3073 93.963 32.373 17.578 1.00 19.66 D MOTA 0 LEU D 13 95.221 32.969 19.344 1.00 20.75 D MOTA 3074 N LEU D 13 96.471 32.949 18.600 1.00 22.59 3075 CA ATOM 3076 CB LEU D 13 18.234 1.00 24.32 MOTA 96.841 34.387 3077 CG LEU D 13 98.215 34.672 17.632 1.00 25.29 D ATOM 98.355 33.966 16.289 1.00 24.58 D ATOM 3078 CD1 LEU D 13 CD2 LEU D 13 98.380 36.177 17.475 1.00 23.52 D ATOM 3079 LEU D 13 19.330 97.646 32,290 1.00 22.44 ATOM 3080 C 97.900 32.578 20.494 1.00 24.67 D ATOM 3081 O LEU D 13 98.350 31.397 18.641 1.00 23.69 D ATOM 3082 N TYR D 14 99.535 30.740 19.196 ATOM 3083 CA TYR D 14 1.00 25.57 99.223 19.765 1.00 26.53 29.360 MOTA 3084 СВ TYR D 14 ATOM 3085 CG TYR D 14 100.445 28.712 20.383 1.00 28.87 100.872 29.057 21.668 1.00 28.57 ATOM 3086 CD1 TYR D 14 28.500 22.218 ATOM 3087 CE1 TYR D 14 102.032 1.00 27.29 101.209 27.793 ..19.664 1.00 29.65 ATOM 3088 CD2 TYR D 14 27.235 20.204 1.00 26.94 D MOTA 102.369 3089 CE2 TYR D 14 ATOM 3090 CZ TYR D 14 102.773 27.592 21.477 1.00 27.22 D OH TYR D 14 103.914 27.039 22.008 1.00 29.69 ATOM 3091 100.553 30.574 18.074 1.00 26.73 MOTA TYR D 14 3092 C 100.210 30.128 16.980 1.00 27.22 ATOM 3093 0 TYR D 14 ATOM 3094 GLN D 15 101.800 30.945 18.338 1.00 26.92 102.847 30.820 17.332 1.00 27.70 D MOTA 3095 CA GLN D 15 GLN D 15 103.164 32.179 16.710 1.00 27.39 ATOM 3096 CB 103.534 1.00 27.78 ATOM GLN D 15 17.704 3097 CG 33.251 1.00 27.70 ATOM 3098 CD GLN D 15 103.806 34.590 17.044 103.723 35.638 17.685 1.00 31.07 MOTA 3099 OE1 GLN D 15 D ATOM NE2 GLN D 15 104.142 34.562 15.763 1.00 25.83 3100 104.097 30.222 17.952 1.00 28.40 ATOM 3101 C GLN D 15 104.368 30.416 1.00 28.81 ATOM 19.141 3102 0 GLN D 15 ATOM 3103 N SER D 16 104.852 29.488 17.143 1.00 27.95

ATOM	3104	CA	SER D	16	106.070	28.834	17.611	1.00 28.04	D
MOTA	3105	CB	SER D		106.613	27.887	16.534	1.00 25.04	D
MOTA	3106	OG	SER D	16	106.879	28.581	15.330	1.00 26.28	D
MOTA	3107	C	SER D	16	107.155	29.824	18.024	1.00 27.77	D
MOTA	3108	0	SER D		107.922	29.558	18.946	1.00 26.81	Ð
ATOM	3109	N	TYR I		107.221	30.965	17.351	1.00 29.70	D
ATOM	3110	CA	TYR D		108.228	31.953	17.694	1.00 32.41	D
ATOM	3111	CB	TYR I		108.248	33.086	16.672	1.00 35.15	D D
ATOM	3112	CG	TYR I		109.440 110.719	33.986 33.556	16.864 16.508	1.00 40.80 1.00 43.28	D
ATOM ATOM	3113 3114		TYR I		111.836	34.345	16.743	1.00 44.62	D
MOTA	3115		TYR I		109.308	35.235	17.460	1.00 40.97	D
ATOM	3116	CB2	TYR I		110.419	36.032	17.702	1.00 44.83	D
ATOM	3117	CZ	TYR I		111.679	35.580	17.341	1.00 45.74	D
ATOM	3118	OH	TYR I		112.788	36.353	17.590	1.00 49.39	D
ATOM	3119	C	TYR I	17	107.954	32.525	19.084	1.00 33.13	D
A'TOM	3120	0	TYR I	17	106.888	33.092	19.332	1.00 32.77	D
MOTA	3121	N	GLY I	18	108.930	32.383	19.981	1.00 32.74	D
ATOM	3122	CA	GLY I		108.780	32.867	21.341	1.00 31.76	D
ATOM	3123	С	GLY I		108.958	31.716	22.311	1.00 32.63	D
ATOM	3124	0	GLY I		110.005	31.600	22.948	1.00 34.20	D
MOTA	3125	И	PRO I		107.946	30.840	22.452 23.256	1.00 33.13	D D
ATOM	3126	CD CA	PRO I		108.029 106.663	29.606 30.906	21.741	1.00 32.71	D
MOTA MOTA	3127 3128	CB	PRO I		106.115	29.492	21.903	1.00 33.20	ã
ATOM	3129	CG	PRO I		106.591	29.128	23.280	1.00 31.76	D
ATOM	3130	C	PRO I		105.768	31.948	22.406	1.00 32.52	D
ATOM	3131	ō	PRO I		105.970	32.282	23.568	1.00 33.11	D
MOTA	3132	N	SER I		104.786	32.463	21.676	1.00 31.92	D
MOTA	3133	CA	SER I	20	103.886	33.455	22.246	1.00 30.99	D
ATOM	3134	CB	SER I	20	104.287	34.867	21.795	1.00 30.92	D
MOTA	3135	OG	SER I		104.263	34.988	20.381	1.00 33.16	D
MOTA	3136	С	SER I		102.441	33.172	21.852	1.00 30.01	D D
ATOM	3137	0	SER I		102.179	32.428 33.763	20.902 22.598	1.00 29.42 1.00 27.60	ם
ATOM	3138	N CA	GLY I		101.512 100.101	33.763	22.338	1.00 27.00	D
ATOM ATOM	3139 3140	C	GLY I		99.309	34.836	22.632	1.00 24.66	D
ATOM	3141	ŏ	GLY I		99.848	35.798	23.187	1.00 23.84	D
ATOM	3142	N	GLN I		98.030	34.834	22.268	1.00 22.55	D
ATOM	3143	CA	GLN I		97.149	35.974	22.527	1.00 20.16	D
MOTA	3144	СВ	GLN 1	D 22	97.301	37.049	21.445	1.00 18.28	D
MOTA	3145	CG	GLN I		96.416	38.284	21.672	1.00 18.60	D
ATOM	3146	CD	GLN I		96.513	39.327	20.562	1.00 18.36	D D
MOTA	3147		GLN :		97.379 95.617	40.207 39.232	20.587 19.582	1.00 19.82 1.00 17.69	D
ATOM ATOM	3148 3149	C	GLN :		95.699	35.517	22.561	1.00 18.61	D
ATOM	3150	Ö	GLN :		95.301		21.790	1.00 17.26	ם
ATOM	3151	N	TYR		94.926	36.097	23.475	1.00 16.42	D
ATOM	3152	CA	TYR		93.507	35.785	23.592	1.00 16.21	D
MOTA	3153	CB	TYR :	D 23	93.212	34.839	24.762	1.00 14.97	D
MOTA	3154	CG	TYR :		91.750	34.438	24.798	1.00 14.24	D
ATOM	3155		TYR		91.309		24.109	1.00 14.49	D
MOTA	3156		TYR		89.969		24.029	1.00 14.23	D
MOTA	3157		TYR		90.795		25.421	1.00 13.21 1.00 13.08	D D
MOTA	3158		TYR		89.443 89.039		25.344 24.647	1.00 13.08	ם
MOTA MOTA	3159 3160	CZ	TYR TYR		87.710		24.566	1.00 16.44	ם
MOTA	3161	C	TYR		92.751		23.806	1.00 15.56	D
ATOM	3162	ŏ	TYR				24.763	1.00 16.57	a
ATOM	3163	N	THR				22.914	1.00 14.11	D
MOTA	3164	CA	THR	D 24	91.026	38.598	22.995	1.00 13.31	D
MOTA	3165	CB	THR	D 24			22.071	1.00 16.07	D
MOTA	3166		THR				20.734	1.00 17.94	D
MOTA	3167		THR				22.514	1.00 13.19	D
ATOM	3168	C	THR				22.519	1.00 12.68	D D
ATOM	3169	0	THR				21.994 22.727	1.00 15.13 1.00 13.47	Ď
MOTA MOTA	3170 3171	N CA	HIS HIS				22.229	1.00 13.47	Ď
ATOM	3172	CB	HIS				23.346	1.00 11.26	D
ATOM	3173	CG	HIS				23.785	1.00 14.42	D
ATOM	3174		HIS				23.723	1.00 12.09	ם
ATOM	3175		L HIS				24.392	1.00 15.93	D
ATOM	3176		L HIS				24.685	1.00 14.24	D C
MOTA	3177	NE	2 HIS	D 2	86.089	35.591	24.289	1.00 13.67	U

ATOM	3178	C	HIS	D	25	87.158	40.495	21.436	1.00 13.30	D
ATOM	3179	0	HIS	D	25	87.573	41.563	21.859	1.00 13.77	D
ATOM	3180	N	GLU		26	86.544	40.376	20.271	1.00 15.40	D
ATOM		CA								
	3181		GLU		26	86.318	41.540	19.434	1.00 16.53	D
MOTA	3182	CB	GLU	D	26	87.109	41.396	18.133	1.00 14.47	D
ATOM	3183	CG	GLU	D	26	88.627	41.460	18.277	1.00 14.81	D
ATOM	3184	CD	GLU	D	26	89.341	41.205	16.947	1.00 19.22	D
ATOM	3185		GLU		26	88.726	41.429	15.884	1.00 22.84	D
ATOM	3186		GLU		26	90.512	40.792	16.953	1.00 17.41	D
MOTA	3187	C	GLU	D	26	84.841	41.721	19.111	1.00 17.28	D
ATOM	3188	0	GLU	D	26	84.073	40.760	19.100	1.00 16.62	D
ATOM	3189	N	PHE	D	27	84.455	42.971	18.879	1.00 19.63	D
ATOM	3190	CA	PHE	D	27	83.092	43.313	18.494	1.00 19.71	D
ATOM	3191	CB	PHE		27					
						82.231	43.722	19.684	1.00 21.05	Œ
ATOM	3192	CG	PHR		27	80.758	43.816	19.348	1.00 24.29	D
ATOM	3193	CD1	PHE	D	27	79.971	42.668	19.278	1.00 23.22	D
ATOM	3194	CD2	PHE	D	27	80.169	45.047	19.073	1.00 22.47	D
ATOM	3195	CB1	PHE	D	27	78.617	42.744	18.940	1.00 24.89	D
ATOM	3196		PHE		27	78.818	45.132	18.733	1.00 24.72	Ď
MOTA	3197	CZ	PHE		27	78.041	43.980	18.667	1.00 22.80	D
ATOM	3198	С	PHE	D	27	83.182	44.482	17.532	1.00 18.41	D
ATOM	3199	0	PHE	D	27	83.700	45.545	17.879	1.00 19.21	D
ATOM	3200	N	ASP	D	28	82.680	44.272	16.321	1.00 18.46	D
ATOM	3201	CA	ASP		28	82.700	45.284	15.272	1.00 18.63	D
ATOM	3202	CB	ASP		28	81.702	46.404	15.568	1.00 19.29	D
ATOM	3203	CG	ASP	D	28	80.268	45.981	15.305	1.00 22.52	D
ATOM	3204	OD1	ASP	D	28	80.076	44.885	14.738	1.00 23.13	D
ATOM	3205	OD2	ASP	D	28	79.333	46.736	15.651	1.00 24.61	D
ATOM	3206	C	ASP		28	84.075	45.865	15.037	1.00 17.83	D
ATOM		ō	ASP		28	84.225	47.069	14.860	1.00 20.60	D
	3207									
ATOM	3208	N	GLY		29	85.079	44.997	15.042	1.00 18.44	D
MOTA	3209	CA	GLY	Ð	29	86.439	45.431	14.788	1.00 19.49	D
ATOM	3210	C	GLY	D	29	87.218	46.011	15.949	1.00 18.93	D
ATOM	3211	0	GLY	D	29	88.382	46.359	15.784	1.00 19.51	D
ATOM	3212	N	ASP		30	86.595	46.122	17.117	1.00 17.91	D
MOTA	3213	CA	ASP		30	87.279	46.667	18.288	1.00 17.21	D
ATOM	3214	CB	ASP	D	30	86.499	47.858	18.831	1.00 15.85	D
ATOM	3215	CG	ASP	D	30	86.594	49.060	17.924	1.00 18.96	D
ATOM	3216	OD1	ASP	D	30	87.731	49.515	17.668	1.00 18.56	D
ATOM	3217		ASP		30	85.541	49.544	17.466	1.00 19.00	D
ATOM	3218	С	ASP		30	87.491	45.629	19.389	1.00 17.20	D
ATOM	3219	0	ASP	D	30	86.651	44.763	19.621	1.00 15.68	D
ATOM	3220	N	GLU	D	31	88.629	45.739	20.062	1.00 18.79	D
ATOM	3221	CA	GLU	D	31	89.015	44.829	21.131	1.00 17.52	D
ATOM	3222	СВ	GLU		31	90.531	44.947	21.363	1.00 19.03	D
ATOM	3223	CG	GLU		31	91.074	44.215	22.579	1.00 22.08	D
MOTA	3224	CD	GLU		31	92.596	44.254	22.653	1.00 25.29	D
MOTA	3225	OE1	GLU	D	31	93.198	45.159	22.041	1.00 26.54	D
ATOM	3226	QE2	GLU	D	31	93.193	43.387	23.331	1.00 25.19	D
ATOM	3227	С	GLU	D	31	88.248	45.109	22.421	1.00 17.80	D
ATOM	3228	o	GLU		31	88.360	46.195	23.004	1.00 16.81	D
					32	87.478		22.862		D
ATOM	3229	N	GLN				44.118		1.00 15.25	
ATOM	3230	CA	GLN		32	86.685	44.230	24.085	1.00 15.53	D
MOTA	3231	CB	GLN	D	32	85.502	43.260	24.044	1.00 12.86	D
MOTA	3232	CG	GLN	D	32	84.391	43.680	23.101	1.00 13.72	D
MOTA	3233	CD	GLN	D	32	83.233	42.708	23.111	1.00 16.53	D
MOTA	3234		GLN		32	83.407	41.526	22.838	1.00 20.27	D
ATOM	3235		GFN		32	82.044	43.203	23.423	1.00 17.48	D
ATOM	3236	С	GLN		32	87.528	43.956	25.329	1.00 16.00	D
ATOM ·	3237	0	GLN	D	32	87.356	44.603	26.366	1.00 15.18	D
MOTA	3238	N	PHE	D	33	88.423	42.981	25.222	1.00 16.17	D
MOTA	3239	CA	PHE		33	89.315	42.638	26.321	1.00 15.74	D
			PHE			88.520	42.083	27.515	1.00 15.40	D
ATOM	3240	CB			33					
ATOM	3241	CG	PHE		33	87.969	40.693	27.307	1.00 15.83	D
MOTA	3242		PHE		33	88.781	39.572	27.480	1.00 16.23	D
ATOM	3243	CD2	PHE	D	33	86.625	40.503	26.977	1.00 17.27	D
ATOM	3244		PHB		33	88.262	38.282	27.332	1.00 15.79	D
ATOM	3245		PHB		33	86.088	39.218	26.827	1.00 15.20	D
ATOM		CZ	PHB		33	86.909	38.108	27.006	1.00 17.77	D
	3246									
MOTA	3247	C	PHE		33	90.330	41.614	25.860	1.00 15.28	D
MOTA	3248	0	PHE		33	90.157	40.979	24.825	1.00 15.16	D
MOTA	3249	N	TYR	D	34	91.405	41.476	26.620	1.00 15.54	D
ATOM	3250	CA	TYR		34	92.414	40.480	26.314	1.00 16.00	D
ATOM	3251	СВ	TYR		34	93.649	41.124	25.670	1.00 17.46	D
				_						

94.508 41.970 26.588 1.00 20.90 ATOM 3252 CG TYR D 34 95.488 41.390 27.391 1.00 21.91 MOTA 3253 CD1 TYR D 34 D ATOM 96.295 42.174 28.221 1.00 24.17 3254 CR1 TYR D 34 94.351 26.638 1.00 20.26 43.354 ATOM 3255 CD2 TYR D 34 TYR D 95.147 44.141 27.463 1.00 24.97 ATOM 3256 CE2 34 ATOM 3257 CZ TYR D 96.117 43.546 28.251 1.00 23.87 34 96.904 44.326 29.065 1.00 26.29 MOTA 3258 OH TYR D 34 27.642 1.00 16.56 MOTA 3259 C TYR D 34 92.766 39.836 1.00 15.36 MOTA 3260 O TYR D 34 92.476 40.386 28.699 93.354 38.653 27.586 1.00 18.29 MOTA 3261 N VAL D 35 28.795 1.00 19.11 CA VAL D 35 93.768 37.971 ATOM 3262 ATOM 3263 CB VAL D 35 93.257 36.514 28.842 1.00 17.61 D ATOM CG1 VAL D 35 93.910 35.780 29.992 1.00 17.99 D 3264 3265 CG2 VAL D 35 91.744 36.493 29.003 1.00 17.82 ATOM 37.950 95,290 28.813 1.00 19.96 ATOM 3266 C VAL D 35 VAL D 35 95.914 37.492 27.866 1.00 17.73 D MOTA 3267 0 38.473 29.880 1.00 22.63 MOTA 3268 N ASP D 36 95.883 97.333 38.456 30.005 1.00 24.79 MOTA ASP D 36 3269 CA 1.00 26.41 31.106 MOTA 3270 CB ASP D 36 97.795 39.409 31.131 1.00 30.12 D ATOM 3271 CG ASP D ,36 99.298 39.574 100.002 38.547 31.252 1.00 32.04 n MOTA 3272 OD1 ASP D 36 1.00 32.20 OD2 ASP D 36 99.776 40.726 31.028 ATOM 3273 30.389 1.00 25.23 ASP D 36 97.650 37.011 MOTA 3274 С 31.502 1.00 25.21 3275 ASP D 36 97.349 36.575 D MOTA 0 98.236 36.272 29.455 1.00 23.64 3276 N LEU D 37 ATOM 29.676 1.00 25.25 LEU D 37 98.549 34.870 ATOM 3277 CA 98.992 34.232 28.355 1.00 21.08 MOTA 3278 CB LEU D 37 27.225 1.00 20.24 D 3279 CG LEU D 37 97.955 34.360 MOTA 37 98.568 33.934 25.899 1.00 17.23 D MOTA 3280 CD1 LEU D 27.541 1.00 19.11 3281 CD2 LEU D 37 96.730 33.516 ATOM 34.626 30.770 1.00 27.73 LEU D 37 99.590 ATOM 3282 C 33.682 31.554 1.00 27.92 D 3283 LEU D 37 99.464 MOTA 0 100.608 35.474 30.837 1.00 29.31 D MOTA 3284 N GLY D 38 GLY D 38 101.629 35.292 31.851 1.00 30.44 D 3285 CA MOTA 35.640 33.242 1.00 32.52 101.141 MOTA 3286 С GLY D 38 D 34.986 34.220 1.00 34.37 MOTA 3287 0 GLY D 38 101.502 MOTA 3288 N ARG D 39 100.309 36.669 33.335 1.00 35.10 D 34.623 1.00 36.92 D CA ARG D 39 99.786 37.103 MOTA 3289 99.693 38.632 34.653 1.00 39.96 D ARG D 39 ATOM 3290 CB 34.301 1.00 44.57 MOTA 3291 CG ARG D 39 101.011 39.318 101.006 40.798 34.667 1.00 49.71 D 3292 CD ARG D 39 MOTA 34.270 1.00 53.08 ם ARG D 39 102.240 41.484 ATOM 3293 NE 34.698 1.00 55.33 103.460 41.164 ATOM 3294 CZ ARG D 39 1.00 56.98 D NH1 ARG D 39 103.635 40.158 35.546 ATOM 3295 104.512 41.859 34.282 1.00 56.80 D ATOM 3296 NH2 ARG D 39 36.476 34.924 1.00 35.86 D 98.429 ARG D 39 MOTA 3297 C 36.022 1.00 35.27 MOTA 3298 O ARG D 39 97.886 36.630 33.944 1.00 34.51 D LYS D 40 97.893 35.757 MOTA 3299 N 96.602 35.095 34.090 1.00 33.49 D LYS D 40 MOTA 3300 CA 35.088 1.00 34.77 D LYS D 40 96.714 33.939 CB ATOM 3301 95.482 33.040 35.133 1.00 41.38 TAYS D 40 ATOM 3302 CG 95.703 31.839 36.046 1.00 45.02 œ LYS D 40 ATOM 3303 1.00 46.54 D LYS D 40 94.443 31.001 36.185 ATOM 3304 CE 1.00 48.98 94.652 29.853 37.112 D ATOM 3305 NZ LYS D 40 1.00 30.95 D LYS D 40 95.511 36.064 34.542 ATOM 3306 С 1.00 28.23 94.780 35.794 35.492 MOTA 3307 0 LYS D 40 33.858 1.00 30.54 D GLU D 41 95.401 37.197 MOTA 3308 N 3309 CA GLU D 41 94.384 38.175 34.210 1.00 30.41 D MOTA 94.980 39.302 35.078 1.00 34.10 D GLU D 41 MOTA 3310 CB 96.180 40.034 34,488 1.00 41.52 D CG GLU D 41 ATOM 3311 1.00 45.72 D MOTA 3312 CD GLU D 41 96.834 40.997 35.482 1.00 48.68 OE1 GLU D 41 97.826 41.665 35.108 D ATOM 3313 1.00 47.60 D OB2 GLU D 41 96.362 41.086 36.638 MOTA 3314 1.00 28.03 93.651 38.766 33.014 ATOM 3315 C GLU D 41 1.00 25.49 ATOM 3316 0 GLU D 41 94.220 38.981 31.940 42 92.364 39.006 33,226 1.00 25.48 MOTA N THR D 3317 THR D 42 91.488 39.582 32.224 1.00 23.42 D ATOM 3318 CA 1.00 22.07 ם 90.035 39.187 32.511 42 ATOM 3319 CB THR D 1.00 18.54 3320 OG1 THR D 42 89.927 37.761 32.468 MOTA 1.00 20.32 CG2 THR D 42 89.087 39.817 31.497 ATOM 3321 1.00 22.29 42 91.615 32.301 D THR D 41.098 C ATOM 3322 1.00 21.54 42 91.492 41.680 33.373 ATOM 3323 0 THR D 1.00 21.50 D VAL D 43 91.874 41.736 31.167 3324 N ATOM 92.004 43.183 31.136 1.00 19.88 ATOM 3325 CA VAL D 43

ATOM	3326	CB	VAL	D	43	93.428	43.584	30.697	1.00 21.56	D
ATOM	3327	CG1	VAL		43	93.620	45.091	30.828	1.00 20.99	D
MOTA	3328	CG2	VAL		43	94.456	42.827	31.539	1.00 19.79	D
MOTA	3329	C	AŸT		43	90.968	43.744	30.164	1.00 20.50	D D
MOTA	3330	0	VAL		43	91.045 89.987	43.513 44.466	28.959 30.690	1.00 19.49 1.00 21.49	D
ATOM ATOM	3331 3332	N CA	TRP		44 44	88.946	45.028	29.836	1.00 22.88	D
ATOM	3333	CB	TRP		44	87.685	45.326	30.649	1.00 21.57	D
ATOM	3334	CG	TRP		44	87.167	44.129	31.372	1.00 21.99	D
MOTA	3335		TRP		44	86.280	43.125	30.854	1.00 22.20	D
MOTA	3336	CE2	TRP	D	44	86.119	42.150	31.862	1.00 22.19	D
MOTA	3337	CE3	TRP	D	44	85.611	42.951	29.634	1.00 20.96	D
MOTA	3338		TRP		44	87.492	43.736	32.633	1.00 23.17	D
MOTA	3339	NE1			44	86.868	42.548	32.937	1.00 23.70	D D
ATOM	3340	CZ2	TRP		44	85.311	41.016 41.824	31.693 29.461	1.00 24.30 1.00 22.81	D
ATOM ATOM	3341 3342	CZ3	TRP		44 44	84.807 84.666	40.870	30.487	1.00 24.05	D
MOTA	3343	Ç	TRP		44	89.425	46.291	29.143	1.00 23.92	D
ATOM	3344	ō	TRP		44	90.081	47.131	29.759	1.00 24.50	D
ATOM	3345	N	CYS		45	89.098	46.417	27.859	1.00 24.24	D
MOTA	3346	CA	CYS	D	45	89.498	47.580	27.069	1.00 26.23	ם
ATOM	3347	CB	CYS		45	89.951	47.141	25.672	1.00 25.96	D
ATOM	3348	SG	CYS		45	91.422	46.098	25.665	1.00 25.42	D
ATOM	3349	C	CYS		45	88.377	48.608	26.950 26.549	1.00 27.07 1.00 28.23	D D
ATOM	3350	0	CYS		45 46	88.612 87.157	49.749 48.193	27.273	1.00 27.18	D
ATOM ATOM	3351 3352	N CA	LEU		46	86.002	49.087	27.232	1.00 28.16	D
ATOM	3353	CB	LEU		46	84.907	48.525	26.320	1.00 27.82	D
ATOM	3354	CG	LEU		46	84.142	49.460	25.372	1.00 30.22	D
ATOM	3355		LEU	D	46	82.792	48.827	25.040	1.00 29.72	D
MOTA	3356	CD2	TEA	D	46	83.928	50.827	25.994	1.00 31.10	D
MOTA	3357	C	LEU		46	85.504	49.138	28.675	1.00 28.73	D
ATOM	3358	0	LEU		46	85.049	48.133	29.216	1.00 28.92 1.00 29.35	D D
ATOM	3359	И	PRO		47	85.601	50.309 51.554	29.318 28.717	1.00 28.33	D
MOTA	3360	CD	PRO PRO		47 47	86.116 85.182	50.533	30.709	1.00 29.01	ם
MOTA MOTA	3361 3362	CA CB	PRO		47	85.139	52.051	30.806	1.00 29.32	D
ATOM	3363	CG	PRO		47	86.307	52.447	29.929	1.00 30.61	D
ATOM	3364	C	PRO		47	83.879	49.875	31.169	1.00 28.51	D
MOTA	3365	0	PRO	D	47	83.867	49.151	32.163	1.00 28.22	D
ATOM	3366	N	VAL		48	82.784	50.126	30.458	1.00 28.05	D
MOTA	3367	CA	VAL		48	81.492	49.545	30.826	1.00 27.41	D D
MOTA	3368	CB	VAL		48	80.406	49.918	29.810 30.027	1.00 26.31 1.00 30.25	D
ATOM	3369		VAI VAI		48 48	79.955 80.949	51.345 49.744	28.398	1.00 26.11	D
ATOM ATOM	3370 3371	CG2 C	VAL		48	81.490	48.022	30.961	1.00 26.77	D
ATOM	3372	ŏ	VAI		48	80.622	47.462	31.627	1.00 27.43	D
MOTA	3373	N	LEU		49	82.449	47.353	30.332	1.00 25.75	D
ATOM	3374	CA	PEC	J D	49	82.517	45.898	30.395	1.00 27.21	D
MOTA	3375	CB	LEU	D	49	83.237	45.354	29.153	1.00 27.47	D
MOTA	3376	CG	LEU		49	82.405	44.886	27.944	1.00 29.74	D
ATOM	3377		LLE		49	81.361	45.898	27.578	1.00 29.28	D
ATOM	3378		2 LEC		49	83.329	44.627 45.374	26.753 31.674	1.00 29.72 1.00 27.86	D D
MOTA	3379	C	TE!		49 49	83.185 83.246	44.163	31.900	1.00 25.45	D
MOTA MOTA	3380 3381	N	ARC		50	83.680	46.283	32.508	1.00 29.82	D
ATOM	3382	CA		3 D	50	84.319	45.892	33.768	1.00 32.18	D
ATOM	3383	СВ		3 D	50	84.900	47.105	34.509	1.00 35.49	D
ATOM	3384	CG	AR	g E	50	86.010	47.890	33.824	1.00 40.53	D
MOTA	3385	CD		3 D		86.524	48.968	34.786	1.00 42.89	D
ATOM	3386	NE		3 D		87.297	50.017		1.00 46.26 1.00 46.43	D D
MOTA	3387			3 D		88.484	49.836		1.00 46.42	D
MOTA	3388		1 ARG 2 ARG			89.049 89.100			1.00 43.78	D
MOTA MOTA	3389 3390			GD		83.283			1.00 31.58	D
ATOM	3391			G D		83.631			1.00 31.56	D
ATOM	3392			N D		82.009		34.397	1.00 30.22	D
MOTA	3393			N D	51	80.942			1.00 30.10	D
ATOM	3394			NE		79.610			1.00 31.37	D
MOTA	3395			NI		79.194			1.00 33.44 1.00 37.07	D D
MOTA	3396	CD		NI		77.888			1.00 37.07	D
MOTA	3397		1 GL 2 GL			76.835 77.951				D
MOTA MOTA	3398 3399			NI		80.830				D
ALUM	3373	_				_,,,,,,				

MOTA	3400	0	GLN :		51	80.291	42.721	35.911	1.00 29.09	D
MOTA	3401	N	PHE		52	81.342	42.899	33.935	1.00 28.19	D
ATOM	3402	CA	PHE		52	81.300	41.468	33.676	1.00 26.27	D
MOTA	3403	CB	PHE		52	81.218	41.188	32.178	1.00 25.00	D
MOTA	3404	CG	PHE		52	80.030	41.801	31.513	1.00 23.07	D
MOTA	3405		PHE		52	78.744	41.569	31.999	1.00 22.75	D
ATOM	3406		PHE		52	80.188	42.594	30.380	1.00 23.46	D
MOTA	3407		PHE		52	77.627	42.122	31.364	1.00 21.26	D
ATOM	3408		PHE		52	79.079	43.151	29.735	1.00 21.92	D
ATOM	3409	CZ	PHE		52	77.799	42.913	30.231	1.00 21.69	D
MOTA	3410	C	PHE		52	82.547	40.797	34.217	1.00 27.11	D
MOTA	3411	0	PHE		52	83.477	41.461	34.669	1.00 27.64	D
ATOM	3412	N	ARG		53	82.556	39.471	34.152	1.00 27.25	D
MOTA	3413	CA	ARG		53	83.683	38.672	34.609	1.00 28.31	D
ATOM	3414	CB	ARG		53	83.347	37.976	35.939	1.00 32.75 1.00 40.59	D
ATOM	3415	CG	ARG		53	83.263	38.921	37.143	1.00 40.39	D D
MOTA	3416	CD	ARG		53	82.418	38.325	38.269		D
ATOM	3417	NE	ARG		53	81.007	38.229	37.892 37.808	1.00 52.14 1.00 53.70	D
ATOM	3418	CZ	ARG		53	80.172	39.265 40.493	38.080	1.00 53.70	D
ATOM	3419		ARG		53 53	80.597 78.910	39.071	37.440	1.00 54.61	D
ATOM	3420		ARG		53	84.007	37.624	33.548	1.00 25.73	D
ATOM	3421	C	ARG ARG		53	83.120	37.103	32.875	1.00 23.75	Ď
ATOM	3422	0	PHE		54	85.290	37.335	33.387	1.00 23.47	D
ATOM	3423	N CA	PHE		54	85.716	36.336	32.425	1.00 19.92	D
ATOM	3424 3425	CB	PHE		54	86.159	36.980	31.113	1.00 15.46	D
MOTA MOTA	3426	CG	PHE		54	86.346	35.994	30.007	1.00 17.29	D
ATOM	3427		PHE		54	85.249	35.506	29.303	1.00 15.32	D
ATOM	3428		PHE		54	87.615	35.503	29.701	1.00 15.07	D
ATOM	3429		PHE		54	85.415	34.539	28.309	1.00 16.04	D
ATOM	3430	CE2	PHE		54	87.788	34.535	28.709	1.00 13.99	D
ATOM	3431	cz	PHE		54	86.688	34.055	28.014	1.00 14.35	D
MOTA	3432	C	PHE		54	86.879	35.598	33.055	1.00 18.63	D
MOTA	3433	ō	PHE		54	87.922	36.188	33.329	1.00 19.50	D
ATOM	3434	N	ASP		55	86.676	34.312	33.309	1.00 19.05	D
ATOM	3435	CA	ASP		55	87.689	33.466	33.921	1.00 19.33	D
ATOM	3436	CB	ASP		55	87.084	32.100	34.237	1.00 21.38	D
MOTA	3437	CG	ASP	D	55	88.090	31.138	34.832	1.00 24.95	D
ATOM	3438	OD1	ASP	D	55	89.264	31.528	35.021	1.00 27.01	D
MOTA	3439	OD2	ASP	D	55	87.703	29.985	35.112	1.00 27.48	D
MOTA	3440	C	ASP	D	55	88.863	33.323	32.955	1.00 19.84	D
MOTA	3441	0	ASP	D	55	88.741	32.691	31.904	1.00 18.07	D
MOTA	3442	N	PRO	D	56	90.024	33.909	33.311	1.00 19.36	a
MOTA	3443	CD	PRO	D	56	90.285	34.584	34.593	1.00 16.09	D
ATOM	3444	CA	PRO		56	91.240	33.867	32.486	1.00 18.34	D
MOTA	3445	CB	PRO		56	92.228	34.729	33.278	1.00 19.78	D
MOTA	3446	CG	PRO		56	91.792	34.517	34.692	1.00 18.66	D
MOTA	3447	C	PRO		56	91.770	32.468	32.206	1.00 18.30	D
MOTA	3448	0	PRO		56	92.583	32.277	31.299	1.00 17.41	D
MOTA	3449	N	GTN		57	91.304	31.489	32.977	1.00 18.31 1.00 18.39	D D
MOTA	3450	CA	GLN		57	91.744	30.114	32.781 33.963	1.00 19.94	D
MOTA	3451	CB	GLN		57	91.314 91.738	29.233 27.773	33.856	1.00 18.50	D
ATOM	3452	CG	GLN GLN		57 57	93.252	27.603	33.765	1.00 23.86	D
ATOM	3453	CD	GLN		57	94.000	28.110	34.612	1.00 23.68	D
MOTA	3454		GLN		57	93.709	26.885	32.739	1.00 19.56	Œ
ATOM	3455	C	GLN		57	91.174	29.555	31.480	1.00 20.01	D
MOTA MOTA	3456 3457	0	GLN		57	91.733	28.618	30.903	1.00 19.26	D
MOTA	3458	N	PHE		58	90.059	30.113	31.016	1.00 19.19	D
MOTA	3459	CA	PHE		58	89.490	29.629	29.765	1.00 20.37	D
ATOM	3460	СВ	PHE		58	88.178	30.347	29.427	1.00 18.69	D
MOTA	3461	CG	PHE		58	87.587	29.912	28.114	1.00 20.67	D
ATOM	3462		PHE		58	88.040	30.456	26.912	1.00 19.84	D
ATOM	3463		PHE		58	86.640	28.891	28.070	1.00 19.87	D
ATOM	3464		PHE		58	87.562	29.984	25.682	1.00 19.25	D
ATOM	3465		PHE			86.156	28.411	26.844	1.00 20.67	D
ATOM	3466	CZ	PHE			86.623	28.961	25.652	1.00 19.50	D
ATOM	3467	c	PHE			90.508	29.892	28.659	1.00 20.46	D
MOTA	3468	ō	PHE			90.745	29.049	27.790	1.00 20.36	D
ATOM	3469	N	ALA	ם	59	91.115	31.070	28.716	1.00 20.85	D
MOTA	3470	CA	ALA	D.	59	92.111	31.477	27.736	1.00 21.87	D
ATOM	3471	CB	ALA	D	59	92.458	32.959	27.937	1.00 20.20	D
ATOM	3472	C	ALA			93.374	30.618	27.819	1.00 22.41	D
ATOM	3473	0	ALA	D	59	93.877	30.151	26.796	1.00 22.54	D

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ATOM	3474	N	TEA D	60	93.890	30.409	29.030	1.00 21.24	D
MOTA	3475	CA	TEA D	60	95.101	29.601	29.188	1.00 22.31	D
ATOM	3476	CB	TEA D	60	95.501	29.474	30.663	1.00 22.79	D
ATOM	3477	CG	TEA D	60	96.063	30.698	31.393	1.00 25.87	D
ATOM	3478		PEA D		96.455	30.303	32.805	1.00 28.75	D
						31.223	30.670	1.00 28.42	D
ATOM	3479		PEA D		97.270				
MOTA	3480	C	TEO D	60	94.891	28.207	28.617	1.00 21.85	D
ATOM	3481	0	LEU D	60	95.731	27.691	27.875	1.00 22.48	D
ATOM	3482	N	THR D	61	93.763	27.600	28.966	1.00 19.32	D
ATOM	3483	CA	THR D		93.457	26.259	28.489	1.00 20.67	D
							29.158	1.00 20.04	D
ATOM	3484	СВ	THR D		92.175	25.721			
MOTA	3485		THR D		92.419	25.539	30.558	1.00 23.09	D
ATOM	3486	CG2	THR D	61	91.759	24.393	28.546	1.00 21.15	D
ATOM	3487	C	THR D	61	93.283	26.240	26.974	1.00 19.50	D
MOTA	3488	0	THR D	61	93.805	25.363	26.288	1.00 18.76	D
ATOM	3489	N	ASN D		92.565	27.229	26.456	1.00 19.66	D
					92.310	27.300	25.032	1.00 19.00	D
ATOM	3490	CA	ASN D						
ATOM	3491	CB	ASN D		91.356	28.453	24.729	1.00 18.52	D
ATOM	3492	CG	ASN I	62	90.262	28.052	23.760	1.00 20.31	D
ATOM	3493	OD1	ASN I	62	89.726	26.942	23.833	1.00 19.27	D
ATOM	3494	ND2	ASN D	62	89.917	28.952	22.854	1.00 22.25	D
ATOM	3495	C	ASN I		93.599	27.445	24.244	1.00 19.63	D
					93.774	26.788	23.221	1.00 21.16	D
MOTA	3496	0	ASN I						D
MOTA	3497	N	ILE D		94.509	28.290	24.724	1.00 19.68	
ATOM	3498	CA	ILE I	63	95.779	28.481	24.033	1.00 18.76	D
ATOM	3499	CB	ILE I	63	96.587	29.660	24.645	1.00 18.72	D
MOTA	3500	CG2	ILE I	63	97.946	29.780	23.966	1.00 17.99	D
ATOM	3501		IPB I		95.813	30.968	24.471	1.00 17.09	D
					95.507	31.313	23.017	1.00 17.47	D
MOTA	3502		IPE I						D
ATOM	3503	C	ILE I		96.613	27.195	24.094	1.00 18.86	
MOTA	3504	0	ILE I	63	97.354	26.885	23.164	1.00 20.67	D
MOTA	3505	N	ALA I	64	96.497	26.448	25.188	1.00 18.22	D
MOTA	3506	CA	ALA I	64	97.244	25.193	25.316	1.00 20.33	D
ATOM	3507	CB	ALA I		97.039	24.574	26.708	1.00 17.30	D
					96.756	24.232	24.233	1.00 21.38	D
MOTA	3508	С	ALA I						
MOTA	3509	0	ALA 1		97.536	23.459	23.677	1.00 23.44	D
MOTA	3510	N	VAL I	D 65	95.459	24.290	23.940	1.00 21.97	D
MOTA	3511	CA	VAL I	D 65	94.872	23.444	22.910	1.00 22.59	D
ATOM	3512	СВ	VAL I	D 65	93.324	23.570	22.890	1.00 22.30	D
ATOM	3513		VAL I		92.744	22.781	21.728	1.00 17.73	D
					92.747	23.053	24.204	1.00 19.10	D
MOTA	3514	CG2						1.00 23.65	D
MOTA	3515	C	VAL		95.441	23.832	21.541		
MOTA	3516	0	VAL	D 65	95.783	22.961	20.746	1.00 23.24	D
ATOM	3517	N	LEU !	D 66	95.552	25.133	21.271	1.00 25.03	D
ATOM	3518	CA	LEU !	D 66	96.102	25.580	19.991	1.00 26.10	D
MOTA	3519	СВ	LEU I		96.104	27.111	19.870	1.00 23.98	D
	3520	CG	LEU		94.826	27.953	19.969	1.00 25.20	D
ATOM						29.233	19.169	1.00 21.70	D
MOTA	3521		LEU		95.030				D
ATOM	3522		LEU :		93.629	27.211	19.435	1.00 26.16	
ATOM	3523	C	LEU	D 66	97.533	25.078	19.880	1.00 26.24	D
ATOM	3524	0	LEU	D 66	97.971	24.667	18.816	1.00 27.10	D
ATOM	3525	N	LYS	D 67	98.262	25.131	20.989	1.00 27.93	D
MOTA	3526	CA	LYS	D 67	99.642	24.658	21.024	1.00 28.00	D
	3527	СВ	LYS		100.215	24.827	22.437	1.00 27.69	D
MOTA						24.316	22.625	1.00 28.46	D
MOTA	3528	CG	LYS		101.633				D
ATOM	3529	CD	LYS		102.086	24.504	24.069	1.00 30.94	
MOTA	3530	CE	LYS	D 67	103.401	23.791	24.356	1.00 32.95	D
MOTA	3531	NZ	LYS	D 67	104.517	24.279	23.503	1.00 35.64	D
MOTA	3532	C	LYS	D 67	99.642	23.182	20.629	1.00 27.56	D
ATOM	3533	0	LYS	D 67	100.414	22.759	19.767	1.00 27.65	D
	3534	N	HIS		98.761	22.405	21.254	1.00 27.05	D
MOTA						20.982	20.956	1.00 26.31	D
ATOM	3535	CA	HIS		98.665			1.00 27.74	D
MOTA	3536	СВ	HIS		97.600	20.324	21.844		
MOTA	3537	CG			97.356	18.879	21.531	1.00 31.20	D
MOTA	3538	CD:	2 HIS	D 68	97.801	17.748	22.130	1.00 31.26	D
ATOM	3539	ND:	1 HIS	D 68	96.582	18.466	20.465	1.00 32.71	a
MOTA	3540		1 HIS		96.560	17.146	20.423	1.00 31.32	D
	3541		2 HIS		97.292	16.686	21.421	1.00 31.58	D
MOTA							19.483	1.00 25.27	D
MOTA	3542		HIS		98.341	20.757			
MOTA	3543		HIS			19.914	18.830	1.00 25.67	D
MOTA	3544	И	ASN			21.521	18.959	1.00 22.00	D
MOTA	3545	CA	ASN	D 69	96.986	21.398	17.561	1.00 23.20	D
ATOM	3546		ASN	D 69		22.210	17.307	1.00 23.27	ם
MOTA	3547					21.504	17.805	1.00 24.20	D
WT OLD	3341								

Amou	2540	ODI	ASN I		c0	94.521	20.536	18.562	1.00 26.69	D
ATOM	3548				59 50				1.00 21.03	D
ATOM	3549		ASN I		69	93.283	21.994	17.381		
ATOM	3550	С	ASN I		69	98.091	21.855	16.601	1.00 24.52	D
MOTA	3551	0	ASN I	0 (69	98.329	21.223	15.570	1.00 22.82	D
MOTA	3552	N	LEU I	י ס	70	98.763	22.954	16.934	1.00 24.56	D
ATOM	3553	CA	LEU I	D '	70	99.831	23.459	16.078	1.00 26.89	D
MOTA	3554	CB	LEU I	ο .	70	100.478	24.707	16.690	1.00 23.85	D
MOTA	3555	CG	LEU I		70	101.619	25.306	15.857	1.00 22.71	D
					70	101.082	25.776	14.519	1.00 19.18	D
MOTA	3556		TEO 1							D
ATOM	3557		LEU !		70	102.254	26.472	16.592	1.00 23.62	
MOTA	3558	C	TEO 1		70	100.900	22.388	15.882	1.00 28.63	D
MOTA	3559	0	TEO 1	D '	70	101.413	22.210	14.780	1.00 27.56	D
MOTA	3560	N	ASN I	D '	71	101.224	21.687	16.967	1.00 31.13	D
ATOM	3561	CA	ASN :	D	71	102.238	20.637	16.962	1.00 35.25	D
ATOM	3562	СВ	ASN :		71	102.393	20.052	18.370	1.00 35.30	D
	3563	CG	ASN I		71	103.149	20.978	19.307	1.00 38.03	D
ATOM							20.751	20.518	1.00 40.05	D
ATOM	3564		ASN :		71	103.197				Ď
MOTA	3565		ASN :		71	103.752	22.026	18.748	1.00 38.78	
MOTA	3566	C	ASN :	D	71	101.931	19.521	15.975	1.00 36.85	D
MOTA	3567	0	ASN	D	71	102.829	18.997	15.316	1.00 36.91	D
MOTA	3568	N	SER	D	72	100.660	19.157	15.876	1.00 38.08	D
ATOM	3569	CA	SER	D	72	100.261	18.104	14.961	1.00 39.44	D
ATOM	3570	СВ	SER		72	98.847	17.623	15.306	1.00 40.69	D
						98.529	16.427	14.611	1.00 44.84	D
MOTA	3571	OG	SER		72				1.00 39.55	D
MOTA	3572	С	SER		72	100.320	18.614	13.520		
ATOM	3573	0	SER	D	72	100.798	17.915	12.625	1.00 38.61	D
MOTA	3574	N	TEA	D	73	99.846	19.839	13.305	1.00 40.64	D
MOTA	3575	CA	TEO	D	73	99.844	20.443	11.974	1.00 42.19	D
ATOM	3576	CB	LEU	מ	73	99.085	21.768	11.990	1.00 42.17	α
ATOM	3577	CG	LEU		73	97.608	21.700	11.608	1.00 43.12	D
ATOM			LEU		73	96.891	20.664	12.443	1.00 44.19	D
	3578							11.801	1.00 44.59	D
MOTA	3579		LEU		73	96.988	23.072			D
MOTA	3580	C	LEU		73	101.237	20.678	11.407	1.00 43.27	
MOTA	3581	0	LEU	D	73	101.466	20.479	10.215	1.00 43.00	D
MOTA	3582	N	ILE	D	74	102.162	21.116	12.253	1.00 44.60	D
ATOM	3583	CA	ILE	D	74	103.529	21.364	11.812	1.00 46.44	D
ATOM	3584	СВ	ILE		74	104.431	21.770	13.000	1.00 46.31	D
			ILE		74	105.893	21.792	12.571	1.00 46.14	D
ATOM	3585							13.529	1.00 45.97	D
MOTA	3586		ILE		74	103.996	23.140			D
MOTA	3587	CD1	ILE		74	104.683	23.561	14.812	1.00 43.97	
ATOM	3588	C	ΊLΕ	D	74	104.077	20.095	11.166	1.00 48.14	D
MOTA	3589	0	ILE	D	74	104.724	20.147	10.119	1.00 48.28	D
MOTA	3590	N	LYS	D	75	103.800	18.957	11.795	1.00 49.68	D
ATOM	3591	CA	LYS		75	104.252	17.669	11.290	1.00 51.82	D
	3592	СВ	LYS		75	104.060	16.589	12.356	1.00 52.85	D
ATOM					75	104.856	16.839	13.621	1.00 54.78	D
MOTA	3593	ÇG	LYS						1.00 57.28	D
MOTA	3594	æ	LYS		75	104.517	15.831	14.704		
MOTA	3595	CE	LYS	D	75	105.222	16.170	16.010	1.00 58.75	D
MOTA	3596	NZ	LYS	D	75	104.803	15.266	17.116	1.00 59.97	D
MOTA	3597	C	LYS	D	75	103.499	17.276	10.023	1.00 52.37	D
ATOM	3598	0	LYS		75	104.106	17.086	B.972	1.00 52.78	D
ATOM	3599	N	ARG		76	102.177	17.171	10.124	1.00 52.67	D
		CA	ARG		76	101.353	16.783	8.986	1.00 52.67	D
ATOM	3600					99.911	16.546	9.439	1.00 53.54	D
MOTA	3601	CB	ARG		76			10.346	1.00 55.62	D
MOTA	3602	CG	ARG		76	99.764	15.339			
ATOM	3603	CD	ARG		76	98.310	15.011	10.639	1.00 58.29	D
MOTA	3604	NB	ARG	D	76	97.628	16.107	11.319	1.00 61.07	D
MOTA	3605	CZ	ARG	D	76	96.437	16.000	11.900	1.00 62.21	D
MOTA	3606	NH:	L ARG	D	76	95.793	14.840	11.885	1.00 62.71	D
ATOM	3607		ARG		76	95.889	17.055	12.492	1.00 61.94	D
		C	ARG		76	101.375	17.761	7.816	1.00 52.35	D
MOTA	3608							6.817	1.00 52.65	ם
MOTA	3609		ARG		76	100.691	17.550			
MOTA	3610	N	SER		77	102.160	18.824	7.932	1.00 52.02	D
ATOM	3611	CA	SER	D	77	102.255	19.807	6.856	1.00 51.87	D
ATOM	3612	CB	SER	D	77	101.945	21.212	7.379	1.00 50.95	D
ATOM	3613		SER	D	77	102.975	21.668	8.239	1.00 48.11	D
ATOM	3614		SER		77	103.667	19.789	6.287	1.00 52.25	D
			SER		77	104.028	20.633		1.00 51.67	D
MOTA	3615						18.814		1.00 52.79	D
MOTA	3616		ASN		78	104.455			1.00 53.67	D
MOTA	3617				78	105.841	18.675			
MOTA	3618				78	105.912				D
MOTA	3619				78	107.298				D
MOTA	3620	OD	1 ASN	D	78	107.959	17.129			D
MOTA	3621		2 ASN		78	107.732		3.184	1.00 58.05	D

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ATOM	3622	C	asn		78	106.549	19.985	6.632	1.00 52.90	D
ATOM	3623	0	asn	D	78	107.300	20.536	5.826	1.00 53.98	D
ATOM	3624	N	SER	D	79	106.275	20.479	7.835	1.00 51.25	D.
MOTA	3625	CA	SER	D	79	106.856	21.715	8.341	1.00 49.59	D
MOTA	3626	CB	SER		79	108.333	21.498	8.664	1.00 49.69	מ
MOTA	3627	OG	SER		79	108.472	20.604	9.753	1.00 52.23	ם
ATOM	3628	C	SER	D	79	106.711	22.931	7.437	1.00 47.21	D
ATOM	3629	0	SER	D	79	107.699	23.588	7.111	1.00 47.49	D
ATOM	3630	N	THR		80	105.483	23.235	7.032	1.00 44.68	ם
MOTA	3631	CA	THR		80	105.245	24.401	6.189	1.00 43.69	D
MOTA	3632	CB	THR	D	80	103.928	24.274	5.407	1.00 45.12	D
MOTA	3633	OG1	THR	D	80	103.976	23.112	4.570	1.00 47.94	D
MOTA	3634	CG2	THR		80	103.706	25.505	4.541	1.00 44.11	D
							25.634	7.094	1.00 42.94	D
ATOM	3635	С	THR		80	105.166				
ATOM	3636	0	THR	D	80	104.225	25.783	7.874	1.00 41.60	D
ATOM	3637	N	ALA	D	81	106.162	26.510	6.988	1.00 40.39	D
ATOM	3638	CA	ALA	D	81	106.215	27.715	7.804	1.00 37.86	D
ATOM	3639	CB	ALA		81	107.657	28.171	7.958	1.00 39.23	D
										D
ATOM	3640	C	ALA		81	105.372	28.846	7.234	1.00 36.29	
ATOM	3641	0	ALA	D	81	104.988	28.829	6.065	1.00 35.21	D
MOTA	3642	N	ALA	D	82	105.087	29.829	8.079	1.00 34.40	D
MOTA	3643	CA	ALA	D	82	104.294	30.984	7.685	1.00 32.51	D
ATOM	3644	СВ	ALA		82	103.915	31.789	8.920	1.00 32.45	D
									1.00 32.78	
ATOM	3645	C	ALA		82	105.064	31.866	6.707		D
MOTA	3646	0	ALA	D	82	106.294	31.913	6.740	1.00 30.87	Q
ATOM	3647	N	THR	D	83	104.333	32.561	5.839	1.00 32.79	D
ATOM	3648	CA	THR		83	104.940	33.459	4.867	1.00 34.48	D
								3.521	1.00 35.64	ā
MOTA	3649	CB	THR		83	104.195	33.429			
ATOM	3650	OG1	THR		83	104.179	32.094	3.006	1.00 38.88	D
ATOM	3651	CG2	THR	D	83	104.880	34.342	2.521	1.00 35.33	D
ATOM	3652	C	THR	D	83	104.886	34.887	5.401	1.00 35.30	D
MOTA	3653	ō	THR		83	103.827	35.355	5.824	1.00 36.88	D
						106.025			1.00 35.07	Ď
MOTA	3654	N	asn		84		35.575	5.379		
ATOM	3655	CA	asn	D	84	106.095	36.949	5.855	1.00 33.90	D
MOTA	3656	CB	asn	D	84	107.548	37.413	6.010	1.00 34.23	D
MOTA	3657	CG	ASN	D	84	108.351	36.545	6.954	1.00 36.16	D
ATOM	3658		ASN		84	107.895	36.195	8.043	1.00 34.99	D
										D
MOTA	3659		asn		84	109.572	36.205	6.545	1.00 37.40	
ATOM	3660	C	asn	D	84	105.419	37.879	4.865	1.00 34.74	D
ATOM	3661	0	asn	D	84	105.814	37.940	3.699	1.00 35.59	D
ATOM	3662	N	GT.f.		85	104.401	38.599	5.327	1.00 34.09	D
ATOM		CA	GLU		85	103.695	39.561	4.489	1.00 32.99	D
	3663									
MOTA	3664	CB	GLU		85	102.239	39.714	4.939	1.00 35.56	D
MOTA	3665	CG	GLU	D	85	101.370	38.475	4.746	1.00 40.80	D
ATOM	3666	æ	GLU	D	85	101.019	38.215	3.291	1.00 43.32	D
MOTA	3667	OE1	GLU	D	85	100.409	39.104	2.658	1.00 46.21	D
ATOM	3668		GLU		85	101.345	37.119	2.782	1.00 44.58	D
MOTA	3669	C	GLU		85	104.418	40.886	4.681	1.00 31.21	D
ATOM	3670	0	GLU	D	85	105.220	41.024	5.602	1.00 32.36	D
MOTA	3671	N	VAL	D	86	104.140	41.848	3.808	1.00 29.71	D
ATOM	3672	CA	VAL	D	86	104.749	43.170	3.882	1.00 27.94	D
ATOM	3673	СВ	VAL		86	105.079	43.712	2.467	1.00 26.90	D
						105.569	45.166	2.543	1.00 23.11	D
ATOM	3674		. VAL		86					
MOTA	3675	CG2	VAL		86	106.134	42.829	1.821	1.00 24.31	D
ATOM	3676	C	VAL	D	86	103.767	44.114	4.574	1.00 29.81	D
MOTA	3677	0	VAL	D	86	102.658	44.343	4.088	1.00 30.28	D
ATOM	3678	N	PRO		87	104.162	44.666	5.729	1.00 29.08	D
							44.310	6.509	1.00 29.37	D
MOTA	3679	æ	PRO		87	105.356				
MOTA	3680	CA	PRO	ם	87	103.306	45.583	6.485	1.00 30.85	D
MOTA	3681	CB	PRO	Q (87	104.083	45.791	7.786	1.00 30.80	D
MOTA	3682	CG	PRO	D	87	104.878	44.551	7.920	1.00 30.83	D
MOTA	3683	C	PRO		87	103.049	46.907	5.772	1.00 31.43	D
			PRO				47.357	4.968	1.00 31.78	D
MOTA	3684	0			87	103.863				
MOTA	3685	N	GLU		88	101.907	47.517	6.081	1.00 31.85	D
ATOM	3686	CA	GLU	D	88	101.516	48.808	5.521	1.00 32.77	D
ATOM	3687	CB	GL.U	ם ז	88	100.195	48.687	4.744	1.00 35.18	D
MOTA	3688	CG	GLU		88	99.814	49.960	3.987	1.00 43.00	D
								3.205	1.00 46.30	D
MOTA	3689	CD	GLU		88	98.512	49.839			
ATOM	3690		f GTC		88	97.439	49.745	3.837	1.00 47.40	D
MOTA	3691	OE:	GLT	D D	88	98.564	49.840	1.954	1.00 48.25	D
ATOM	3692	C	GL	D	88	101.338	49.748	6.721	1.00 31.26	D
ATOM	3693	ō	GL		88	100.556	49.457	7.630	1.00 31.21	D
		И					50.864	6.728	1.00 28.43	D
ATOM	3694		VAI		89	102.060				
MOTA	3695	CA	VAI	םנ	89	101.988	51.806	7.842	1.00 26.87	D

ATOM	3696	СВ	VAL D	89	103.385	52.024	8.454	1.00 26.58	D
ATOM	3697		VAL D	89	103.277	52.886	9.699	1.00 26.80	ת
ATOM	3698		VAL D	89	104.021	50.679	8.787	1.00 24.58	ם
	3699	C	VAL D	89	101.389	53.174	7.505	1.00 27.02	D
ATOM			VAL D	89	101.698	53.772	6.473	1.00 26.22	ם
MOTA	3700	0					8.394	1.00 26.33	D
MOTA	3701	N	THR D	90	100.530	53.662			D
ATOM	3702	CA	THR D	90	99.881	54.955	8.219	1.00 26.05	
ATOM	3703	CB	THR D	90	98.414	54.802	7.769	1.00 27.24	D
MOTA	3704		THR D	90	98.359	54.063	6.543	1.00 31.41	D
MOTA	3705		THR D	90	97.786	56.163	7.545	1.00 28.57	D
ATOM	3706	C	THR D	90	99.883	55.698	9.546	1.00 24.83	D
MOTA	3707	0	THR D	90	99.542	55.120	10.581	1.00 25.45	D
ATOM	3708	N	VAL D	91	100.266	56.972	9.512	1.00 22.04	ם
ATOM	3709	CA	VAL D	91	100.300	57.791	10.716	1.00 21.50	D
ATOM	3710	CB	VAL D	91	101.749	58.280	11.031	1.00 23.04	D
ATOM	3711	CG1	VAL D	91	· 101.737	59.245	12.225	1.00 22.74	D
MOTA	3712	CG2	VAL D	91	102.650	57.082	11.340	1.00 20.38	ם
ATOM	3713	C	VAL D	91	99.369	58.993	10.553	1.00 21.65	D
ATOM	3714	0	VAL D	91	99.357	59.653	9.509	1.00 21.70	D
ATOM	3715	N	PHE D	92	98.573	59.252	11.586	1.00 21.34	ם
ATOM	3716	CA	PHE D	92	97.633	60.363	11.580	1.00 21.48	D
ATOM	3717	СВ	PHE D	92	96.370	59.985	10.788	1.00 21.60	D
			PHE D	92	95.652	58.771	11.314	1.00 22.22	D
ATOM	3718	CG						1.00 24.10	Ď
ATOM	3719		PHE D	92	94.601	58.902	12.215		
MOTA	3720		DHE D	92	96.038	57.495	10.925	1.00 24.53	D
MOTA	3721		PHE D	92	93.940	57.774	12.724	1.00 22.72	D
ATOM	3722	CE2	PHE D	92	95.386	56.355	11.428	1.00 23.87	D
MOTA	3723	CZ	PHE D	92	94.335	56.501	12.329	1.00 21.18	D
MOTA	3724	С	PHE D	92	97.303	60.700	13.030	1.00 22.72	Q
ATOM	3725	0	PHE D	92	97.607	59.921	13.933	1.00 22.31	D
ATOM	3726	N	SER D	93	96.696	61.859	13.261	1.00 22.45	D
ATOM	3727	CA	SER D	93	96.366	62.262	14.623	1.00 21.69	D
ATOM	3728	CB	SER D	93	96.599	63.764	14.799	1.00 20.96	D
ATOM	3729	OG	SER D	93	95.696	64.508	14.010	1.00 25.08	D
ATOM	3730	C	SER D	93	94.931	61.913	14.990	1.00 21.02	D
MOTA	3731	ō	SER D	93	94.078	61.755	14.127	1.00 20.62	D
MOTA	3732	N	LYS D	94	94.676	61.791	16.283	1.00 20.66	D
ATOM	3733	CA	LYS D	94	93.350	61.453	16.768	1.00 24.11	Ď
ATOM	3734	СВ	LYS D	94	93.444	60.985	18.223	1.00 24.91	D
ATOM	3735	CG	LYS D	94	92.121	60.605	18.865	1.00 29.49	ø
			LYS D	94	92.353	60.101	20.293	1.00 32.97	D
ATOM	3736	CD				59.909	21.052	1.00 33.37	D
MOTA	3737	CE	LYS D	94	91.050	58.897	20.399	1.00 34.08	Ď
MOTA	3738	NZ	LYS D	94	90.175	62.646	16.654	1.00 24.40	Ď
MOTA	3739	C	LYS D	94	92.406		16.356	1.00 24.55	Ď
MOTA	3740	0	LYS D	94	91.224	62.495			Ď
MOTA	3741	N	SER D		92.935	63.834	16.894	1.00 25.54	
MOTA	3742	CA	SER D		92.133	65.040	16.815	1.00 29.22	D
MOTA	3743	CB	SER D		91.932	65.643	18.208	1.00 30.47	D
MOTA	3744	OG	SER D		91.236	64.746	19.060	1.00 36.11	D
ATOM	3745	С	SER D		92.843	66.046	15.932	1.00 29.71	D
MOTA	3746	0	SER D	95	93.993	65.834	15.531	1.00 29.68	D
MOTA	3747	N	PRO D	96	92.159	67.146	15.588	1.00 29.93	D
MOTA	3748	CD	PRO D	96	90.760	67.532	15.843	1.00 31.14	D
ATOM	3749	CA	PRO D	96	92.836	68.129	14.747	1.00 29.29	D
ATOM	3750	CB	PRO D	96	91.714	69.097	14.369	1.00 31.65	D
MOTA	3751	CG	PRO D	96	90.777	69.010	15.545	1.00 30.66	D
ATOM	3752	C	PRO D		93.939	68.765	15.587	1.00 27.35	D
ATOM	3753	o	PRO D		93.818	68.904	16.806	1.00 24.86	D
MOTA	3754	N	VAL D		95.025	69.127	14.929	1.00 26.81	D
ATOM	3755	CA	VAL		96.158	69.706	15.615	1.00 29.25	D
MOTA	3756	CB	VAL I		97.438	69.501	14.783	1.00 31.49	D
MOTA			VALI		98.652	69.998	15.556	1.00 33.50	D
	3757					68.029	14.415	1.00 34.03	D
ATOM	3758		VAL I		97.583			1.00 28.80	D
ATOM	3759	C	VAL I		96.007	71.196	15.910	1.00 28.78	D
MOTA	3760	0	VAL		95.749	71.998	15.012		ם
MOTA	3761	N	THR I		96.144	71.559	17.178	1.00 27.47	
ATOM	3762	CA	THR I		96.091	72.960	17.572	1.00 26.55	D
MOTA	3763	CB	THR I		94.723	73.365	18.209	1.00 26.16	D
MOTA	3764		L THR I		94.684	72.961	19.575	1.00 31.83	D
MOTA	3765	CG2			93.567	72.717	17.469	1.00 23.66	D
ATOM	3766	C	THR I	98	97.220		18.581	1.00 25.73	ם
ATOM	3767	0	THR I	98	97.260		19.591	1.00 27.12	D
ATOM	3768	N	LEU I	99	98.159	74.005	18.285	1.00 26.12	D
ATOM	3769	CA	TEO I		99.307		19.156	1.00 27.47	D

ATOM	3770	CB	TEA D	99	100.089	75.459	18.675	1.00 31.04	D
ATOM	3771	CG	LEU D	99	100.758	75.309	17.310	1.00 33.09	D
ATOM	3772	CD1	LEU D	99	101.458	76.607	16.940	1.00 36.20	D
ATOM	3773		LEU D		101.754	74.165	17.361	1.00 35.56	D
ATOM	3774	C	PEO D		98.935	74.416	20.621	1.00 26.08	D
MOTA	3775	0	TEO D		98.077	75.222	20.946	1.00 25.97	ם
ATOM	3776	N	GLY D	100	99.585	73.654	21.500	1.00 26.97	D
ATOM	3777	CA	GLY D	100	99.310	73.749	22.924	1.00 26.03	D
ATOM	3778	C	GLY D	100	98.233	72.798	23.422	1.00 26.02	D
ATOM	3779	Ó	GLY D		98.020	72.662	24.629	1.00 25.51	D
			GLN D		97.553	72.143	22.491	1.00 25.73	D
ATOM	3780	N							D
ATOM	3781	CA	GLN D		96.490	71.199	22.820	1.00 28.13	
ATOM	3782	CB	GLN I	101	95.372	71.297	21.776	1.00 32.24	D
ATOM	3783	CG	GLN I	101	94.617	69.981	21.560	1.00 38.65	D
ATOM	3784	CD	GLN I	101	94.680	69.459	20,115	1.00 41.08	Œ
ATOM	3785	OEL	GLN I	101	95.760	69.348	19.511	1.00 38.18	D
ATOM	3786	NE2			93.515	69.119	19.566	1.00 40.87	D
		C	GLN I		96.994	69.756	22.861	1.00 25.22	D
ATOM	3787								D
MOTA	3788	0	GLN I		97.477	69.245	21.857	1.00 24.55	
ATOM	3789	N	PRO I	102	96.885	69.078	24.019	1.00 24.18	Ð
ATOM	3790	CD	PRO I	102	96.436	69.544	25.343	1.00 22.22	D
ATOM	3791	CA	PRO I	102	97.359	67.683	24.080	1.00 22.76	D
ATOM	3792	CB	PRO I		96.983	67.253	25.494	1.00 22.02	D
MOTA	3793	CG	PRO I		97.088	68.542	26.274	1.00 22.44	D
								1.00 21.72	ם
MOTA	3794	С	PRO I		96.649	66.845	23.015		
ATOM	3795	0	PRO I		95.429	66.922	22.876	1.00 22.65	D
ATOM	3796	N	asn I	103	97.409	66.055	22.264	1.00 19.84	D
MOTA	3797	CA	asn i	103	96.833	65.225	21.209	1.00 17.89	D
ATOM	3798	CB	ASN I	103	97.112	65.856	19.838	1.00 16.30	D
MOTA	3799	CG	ASN I		96.005	65.587	18.824	1.00 16.50	D
	3800		ASN I		95.552	64.446	18.636	1.00 16.80	D
MOTA									D
MOTA	3801		ASN I		95.569	66.643	18.160	1.00 14.61	
ATOM	3802	C	asn i	103	97.410	63.805	21.248	1.00 17.24	D
ATOM	3803	0	asn i	103	98.199	63.473	22.129	1.00 15.74	D
MOTA	3804	N	ILE I	104	97.010	62.977	20.284	1.00 17.39	D
ATOM	3805	CA	ILE I	104	97.465	61.595	20.198	1.00 15.30	D
ATOM	3806	СВ	ILB I		96.402	60.627	20.755	1.00 17.89	D
					96.818	59.175	20.498	1.00 13.27	D
MOTA	3807	CG2						1.00 18.46	D
MOTA	3808	CG1			96.202	60.886	22.253		
ATOM	3809		ILE I		95.179	59.965	22.895	1.00 17.98	D
MOTA	3810	C	ILE I	104	97.760	61.185	18.763	1.00 17.15	D
ATOM	3811	0	ILE I	104	96.887	61.283	17.902	1.00 18.07	D
MOTA	3812	N	TEO 1	105	98.987	60.727	18.509	1.00 16.66	D
ATOM	3813	CA	LEU I	105	99.370	60.272	17.177	1.00 16.59	D
ATOM	3814	CB	LEU I		100.864	60.482	16.895	1.00 17.56	מ
					101.375	61.926	16.842	1.00 21.66	D
MOTA	3815	CG		105					D
ATOM	3816		LEU		102.811	61.943	16.302	1.00 21.26	
MOTA	3817	CD2	TEO 1	D 105	100.460	62.771	15.951	1.00 21.56	D
MOTA	3818	C	LEU :	D 105	99.061	58.804	17.128	1.00 17.13	D
MOTA	3819	0	LEU I	D 105	99.368	58.056	18.056	1.00 18.35	D
ATOM	3820	N	ILE I	D 106	98.432	58.399	16.039	1.00 17.88	D
ATOM	3821	CA	TIE	D 106	98.045	57.016	15.839	1.00 17.14	D
_	3822	CB		D 106	96.525	56.939	15.492	1.00 16.99	D
MOTA						55.496	15.318	1.00 15.63	D
ATOM	3823		ILE :		96.093				D
ATOM	3824		ILE		95.711	57.619	16.604	1.00 19.04	
MOTA	3825	CDI	ILE	D 106	94.238	57.877	16.260	1.00 16.48	D
MOTA	3826	С	ILE	D 106	98.876	56.431	14.700	1.00 17.19	D
MOTA	3827	0	ILE	D 106	98.941	57.004	13.618	1.00 16.06	D
ATOM	3828	N	CYS	D 107	99.540	55.312	14.966	1.00 18.84	D
ATOM	3829	CA		D 107	100.339	54.637	13.954	1.00 19.74	D
ATOM				D 107	99.634	53.323	13.670	1.00 20.17	D
	3830	C							D
MOTA	3831	0		D 107	99.632	52.421	14.507	1.00 20.08	
MOTA	3832	CB		D 107	101.755	54.349	14.453	1.00 22.00	D
MOTA	3833	SG	CYS	D 107	102.800	53.514	13.211	1.00 28.61	D
MOTA	3834	N	LEU	D 108	99.027	53.221	12.493	1.00 19.48	a
ATOM	3835	CA		D 108	98.313	52.015	12.113	1.00 19.67	D
ATOM	3836	CB.		D 108	97.024	52.391	11.369	1.00 19.98	D
					95.977	51.358	10.925	1.00 20.40	D
ATOM	3837	CG		D 108				1.00 20.15	D
MOTA	3838		I PEO		95.883	51.366	9.412		
MOTA	3839	CD:	S PEA		96.301	49.971	11.454	1.00 19.44	D
MOTA	3840	C	LEU	D 108	99.207	51.145	11.237	1.00 19.84	D
MOTA	3841	0	LEU	D 108	99.657	51.563	10.170	1.00 20.11	D
ATOM	3842	N		D 109	99.473	49.940	11.721	1.00 19.32	D
MOTA	3843	CA		D 109	100.289	48.972	11.016	1.00 19.64	D

MOTA	3844	CB	VAL D 109	101.368	48.402	11.958	1.00 19.40	D
ATOM	3845		VAL D 109		47.474	11.202	1.00 18.01	D
ATOM	3846		VAL D 109		49.560	12.590	1.00 17.30	D
ATOM	3847	C	VAL D 109		47.876	10.568	1.00 21.45	D
ATOM	3848	0	VAL D 109		47.079	11.382 9.274	1.00 22.65 1.00 22.00	D D
ATOM ATOM	3849 3850	N CA	ASP D 110		47.861 46.901	8.689	1.00 23.80	ם
MOTA	3851	CB	ASP D 110		47.648	7.728	1.00 24.68	D
ATOM	3852	CG	ASP D 110		47.002	7.603	1.00 26.64	D
ATOM	3853		ASP D 110		45.915	8.177	1.00 28.80	D
MOTA	3854	OD2	ASP D 110	94.920	47.591	6.926	1.00 27.99	D
ATOM	3855	C	ASP D 110		45.756	7.944	1.00 23.77	D
ATOM	3856	0	ASP D 110		45.831	7.684	1.00 22.82	D
MOTA	3857	N	ASN D 11:		44.711	7.604	1.00 23.55	D
MOTA	3858	CA	ASN D 11:		43.530	6.889	1.00 23.79 1.00 25.36	D
MOTA	3859	CB CG	ASN D 11:		43.867 42.610	5.425 4.562	1.00 25.36	D D
MOTA MOTA	3860 3861		ASN D 11:		42.547	3.724	1.00 29.58	D
ATOM	3862		ASN D 11:		41.611	4.761	1.00 30.51	D
ATOM	3863	C	ASN D 11:		42.941	7.556	1.00 22.70	Ð
ATOM	3864	0	ASN D 11:	100.834	42.784	6.929	1.00 22.97	D
ATOM	3865	N	ILE D 11:	99.656	42.612	8.835	1.00 22.14	D
ATOM	3866	CA	ILE D 11:		42.038	9.598	1.00 20.20	D
ATOM	3867	CB	ILE D 11:		42.536	11.055	1.00 18.82	D
ATOM	3868		ILE D 11:		41.950	11.808	1.00 15.77	D
ATOM	3869		ILE D 11:		44.058	11.103	1.00 19.09 1.00 21.18	D D
ATOM	3870	CDI	ILE D 11:			12.514 9.659	1.00 21.18	D
ATOM ATOM	3871 3872	0	ILE D 11:			10.002	1.00 22.04	D
ATOM	3873	N	PHE D 11:			9.338	1.00 21.35	D
ATOM	3874	CA	PHE D 11			9.409	1.00 19.93	D
ATOM	3875	CB	PHE D 11	100.822	37.726	8.462	1.00 21.28	D
MOTA	3876	CG	PHE D 11			8.825	1.00 20.91	D
MOTA	3877		PHE D 11			9.838	1.00 19.85	D
ATOM	3878		PHE D 11			8.230	1.00 22.61	D D
ATOM	3879		PHE D 11			10.264 8.646	1.00 20.63 1.00 21.21	D
ATOM ATOM	3880 3881	CE2	PHE D 11			9.669	1.00 20.87	D
ATOM	3882	C	PHE D 11			9.071	1.00 19.98	D
ATOM	3883	ŏ	PHE D 11			8.044	1.00 20.80	D
ATOM	3884	N	PRO D 11		37.005	9.925	1.00 21.26	D
MOTA	3885	CD.	PRO D 11	4 105.101	36.414	9.732	1.00 21.94	D
MOTA	3886	CA	PRO D 11			11.166	1.00 21.41	D
MOTA	3887	СВ	PRO D 11			11.625	1.00 21.03	D
MOTA	3888	CG	PRO D 11			11.115 12.185	1.00 22.98 1.00 21.84	D D
MOTA MOTA	3889 3890	C O	PRO D 11 PRO D 11			12.103	1.00 20.41	D
ATOM	3891	N	PRO D 11			13.222	1.00 22.52	ם
ATOM	3892	CD	PRO D 11			13.445	1.00 22.08	D
ATOM	3893	CA	PRO D 11		38.448	14.266	1.00 21.19	D
MOTA	3894	CB	PRO D 11	5 100.730	37.895	15.025	1.00 20.92	D
MOTA	3895	CG	PRO D 11			14.902	1.00 19.88	D
MOTA	3896	C	PRO D 11			15.171	1.00 21.62	D
MOTA	3897	0	PRO D 11			16.356 14.588	1.00 22.92 1.00 21.58	D D
ATOM	3898	N CA	VAL D 11 VAL D 11			15.300	1.00 22.53	D
MOTA MOTA	3899 3900	СВ	VAL D 11			15.067	1.00 24.90	Œ.
ATOM	3901		VAL D 11			15.713	1.00 24.06	D
ATOM	3902		VAL D 11			15.641	1.00 24.88	D
MOTA	3903	C	VAL D 11		40.929	14.708	1.00 21.86	. Д
MOTA	3904	0	VAL D 11			13.509	1.00 20.87	D
MOTA	3905	N	VAL D 11			15.534	1.00 20.65	D
MOTA	3906	CA	VAL D 11			15.007	1.00 21.60	D D
MOTA	3907	CB	VAL D 11			14.345	1.00 18.11	D
ATOM	3908		VAL D 11			15.403 13.469	1.00 17.02	D
MOTA MOTA	3909 3910	C	VAL D 11 VAL D 11			16.092	1.00 23.84	D
ATOM	3911	0	VAL D 1			17.280	1.00 24.78	Ď
ATOM	3912	N	ASN D 1			15.670	1.00 27.93	D
ATOM	3913	CA	ASN D 13			16.593	1.00 30.45	D
ATOM	3914	CB	ASN D 13			16.538	1.00 33.93	D
MOTA	3915	CG	ASN D 11			17.650	1.00 39.88	ם
MOTA	3916		LASN D 1			17.856	1.00 42.45	D D
MOTA	3917	ND	ASN D 1	111.43	B 45.946	18.375	1.00 43.14	ט

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ATOM	3918	C	ASN D 118	107.960	47.465	16.181	1.00 27.72	D
MOTA	3919	0	ASN D 118	108.398	47.952	15.140	1.00 26.88	D
MOTA	3920	N	ILE D 119	107.126	48.113	16.988	1.00 27.59	D
ATOM	3921	CA	ILE D 119	106.680	49.476	16.700	1.00 27.12	D
ATOM	3922	СВ	ILE D 119	105.133	49.580	16.719	1.00 27.17	D
				104.698	50.994	16.346	1.00 26.16	D
ATOM	3923		ILE D 119					
MOTA	3924		ILE D 119	104.528	48.572	15.741	1.00 24.63	D
ATOM	3925	CD1	ILE D 119	103.026	48.423	15.877	1.00 24.19	D
MOTA	3926	C	ILE D 119	107.243	50.436	17.746	1.00 27.72	D
MOTA	3927	0	ILE D 119	107.050	50.248	18.946	1.00 26.86	D
ATOM	3928	N	THR D 120	107.951	51.460	17.291	1.00 27.54	D
				108.524		18.214	1.00 29.37	ם
ATOM	3929	CA	THR D 120		52.423			
MOTA	3930	СВ	THR D 120	110.022	52.131	18.477	1.00 32.22	D
ATOM	3931	OG1	THR D 120	110.722	52.034	17.229	1.00 35.14	D
ATOM	3932	CG2	THR D 120	110.176	50.817	19.247	1.00 35.67	D
ATOM	3933	C	THR D 120	108.369	53.826	17.668	1.00 27.95	D
ATOM	3934	ō	THR D 120	108.398	54.035	16.459	1.00 29.89	D
					54.789	18.560	1.00 26.28	D
ATOM	3935	N	TRP D 121	108.187				
ATOM	3936	CA	TRP D 121	108.031	56.171	18.135	1.00 26.93	D
ATOM	3937	CB	TRP D 121	106.935	56.866	18.940	1.00 24.20	D
MOTA	3938	CG	TRP D 121	105.568	56.343	18.687	1.00 22.03	D
ATOM	3939	CD2		104.643	56.826	17.707	1.00 20.30	D
		CE2		103.454	56.085	17.856	1.00 20.70	D
MOTA	3940							D
ATOM	3941		TRP D 121	104.705	57.817	16.717	1.00 17.15	
MOTA	3942		TRP D 121	104.929	55.351	19.365	1.00 21.06	D
ATOM	3943	NE1	TRP D 121	103.655	55.190	18.875	1.00. 22.39	D
MOTA	3944	CZ2	TRP D 121	102.332	56.305	17.057	1.00 17.25	D
ATOM	3945	CZ3		103.593	58.036	15.924	1.00 17.92	D
			TRP D 121	102.419	57.282	16.099	1.00 19.11	D
MOTA	3946					18.284	1.00 26.88	D
MOTA	3947	C	TRP D 121	109.319	56.957			
MOTA	3948	0	TRP D 121	110.059	56.789	19.251	1.00 27.48	D
ATOM	3949	N	LEU D 122	109.572	57.830	17.321	1.00 29.82	D
ATOM	3950	CA	LEU D 122	110.764	58.658	17.343	1.00 31.91	D
ATOM	3951	CB	LEU D 122	111.664	58.331	16.144	1.00 34.65	D
		CG	LEU D 122	112.391	56.977	16.112	1.00 37.28	D
ATOM	3952				56.828	17.360	1.00 37.11	D
MOTA	3953		LEU D 122	113.247				
MOTA	3954	CD2	LEU D 122	111.394	55.840	16.025	1.00 39.41	D
MOTA	3955	C	LEU D 122	110.416	60.142	17.324	1.00 31.97	D
ATOM	3956	0	LEU D 122	109.619	60.593	16.503	1.00 31.46	D
ATOM	3957	N	SER D 123	111.010	60.889	18.250	1.00 31.03	Q
ATOM	3958	CA	SER D 123	110.813	62.331	18.326	1.00 33.04	D
			SER D 123	110.312	62.745	19.712	1.00 32.42	D
ATOM	3959	CB			64.154	19.793	1.00 32.43	D
MOTA	3960	OG	SER D 123	110.169				Ď
MOTA	3961	С	SER D 123	112.184	62.948	18.062	1.00 33.10	
ATOM	3962	0	SER D 123	113.108	62.784	18.860	1.00 33.57	D
ATOM	3963	N	ASN D 124	112.309	63.646	16.941	1.00 33.51	D
ATOM	3964	CA	ASN D 124	113.575	64.258	16.553	1.00 36.20	D
MOTA	3965	CB	ASN D 124	113.963	65.392	17.510	1.00 34.61	D
	3966	CG	ASN D 124	112.946	66.512	17.531	1.00 34.17	D
MOTA				112.262	66.764	16.539	1.00 34.73	D
MOTA	3967		1 ASN D 124				1.00 35.34	D
MOTA	3968	ND:	2 ASN D 124	112.850	67.202	18.660		
MOTA	3969	С	ASN D 124	114.664	63.191	16.561	1.00 37.34	D
ATOM	3970	0	ASN D 124	115.747	63.401	17.104	1.00 37.93	D
MOTA	3971	N	GLY D 125	114.358	62.039	15.970	1.00 38.73	D
MOTA	3972	CA	GLY D 125	115.317	60.951	15.910	1.00 39.56	D
			GLY D 125	115.457	60.131	17.183	1.00 40.55	D
MOTA	3973	C			59.054	17.157	1.00 42.52	D
ATOM	3974	0	GLY D 125	116.051				D
MOTA	3975	N	HIS D 126	114.911	60.622	18.291	1.00 40.35	
MOTA	3976	CA	HIS D 126	115.009	59.918	19.569	1.00 41.15	D
ATOM	3977	CB	HIS D 126	115.234	60.923	20.702	1.00 43.51	. Б
ATOM	3978	CG		116.525	61.678	20.599	1.00 47.67	Q
			2 HIS D 126	116.775	62.997	20.422	1.00 47.36	D
ATOM	3979			117.757	61.064	20.694	1.00 49.39	D
MOTA	3980		1 HIS D 126				1.00 48.59	D
ATOM	3981		1 HIS D 126	118.709	61.973	20.581		
MOTA	3982	NE	2 HIS D 126	118.140	63.154	20.415	1.00 48.17	D
MOTA	3983	C	HIS D 126	113.794	59.053	19.907	1.00 40.38	D
ATOM	3984		HIS D 126	112.648	59.458	19.706	1.00 39.87	D
ATOM	3985		SER D 127		57.863	20.438	1.00 39.11	D
					56.939	20.821	1.00 39.54	D
MOTA	3986				55.592	21.232	1.00 40.04	D
ATOM	3987						1.00 45.08	D
ATOM	3988				55.001	20.159		
MOTA	3989	C	SER D 127		57.492	21.979	1.00 38.18	D
ATOM	3990	0	SER D 127	112.707	58.054	22.930	1.00 38.52	D
ATOM	3991		VAL D 128		57.326	21.894	1.00 36.40	D

MOTA	3992	CA	VAL D 128	109.967	57.800	22.942	1.00 35.00	D
ATOM	3993	CB	VAL D 128	108.699	58.444	22.358	1.00 33.68	D
ATOM	3994	CG1	VAL D 128	107.834	59.001	23.479	1.00 32.31	D
MOTA	3995		VAL D 128	109.081	59.543	21.383	1.00 32.69	D
			VAL D 128	109.574	56.608	23.790	1.00 34.62	D
MOTA	3996	C					1.00 35.98	Ď
MOTA	3997	0	VAL D 128	109.150	55.584	23.268		
ATOM	3998	N	THR D 129	109.715	56.743	25.100	1.00 35.57	D
MOTA	3999	CA	THR D 129	109.393	55.653	26.007	1.00 38.21	ם
ATOM	4000	CB	THR D 129	110.562	55.410	26.992	1.00 40.63	D
ATOM	4001	OG1	THR D 129	110.184	54.413	27.949	1.00 44.78	D
ATOM	4002		THR D 129	110.929	56.700	27.715	1.00 42.66	D
ATOM	4003	c	THR D 129	108.103	55.862	26.799	1.00 36.54	D
			THR D 129	107.359	54.911	27.042	1.00 38.87	D
ATOM	4004	0					1.00 33.00	Ď
MOTA	4005	N	GLU D 130	107.833	57.101	27.195		
MOTA	4006	CA	GLU D 130	106.631	57.401	27.963	1.00 31.03	D
MOTA	4007	CB	GLU D 130	106.935	58.453	29.039	1.00 33.90	D
ATOM	4008	CG	GLU D 130	108.067	58.089	29.987	1.00 38.08	D
ATOM	4009	æ	GLU D 130	107.809	56.788	30.731	1.00 43.43	Ø
ATOM	4010		GLU D 130	106.744	56.672	31.375	1.00 45.61	D
	4011		GLU D 130	108.671	55.879	30.675	1.00 45.67	D
ATOM				105.521	57.922	27.058	1.00 27.87	D
ATOM	4012	C	GLU D 130				1.00 24.56	D
ATOM	4013	0	GLU D 130	105.795	58.527	26.029		
MOTA	4014	N	GLY D 131	104.272	57.692	27.457	1.00 26.29	D
MOTA	4015	CA	GLY D 131	103.140	58.166	26.679	1.00 25.19	D
MOTA	4016	С	GLY D 131	102.826	57.304	25.474	1.00 24.46	D
MOTA	4017	0	GLY D 131	102.130	57.725	24.559	1.00 23.65	D
ATOM	4018	N	VAL D 132	103.349	56.089	25.476	1.00 22.83	D
ATOM	4019	CA	VAL D 132	103.117	55.169	24.379	1.00 23.04	D
		CB	VAL D 132	104.448	54.674	23.784	1.00 22.91	D
ATOM	4020						1.00 24.12	D
MOTA	4021		VAL D 132	104.182	53.538	22.821		
MOTA	4022	CG2		105.164	55.816	23.076	1.00 22.85	D
ATOM	4023	C	VAL D 132	102.326	53.943	24.829	1.00 21.91	D
ATOM	4024	0	VAL D 132	102.535	53.416	25.917	1.00 21.27	D
ATOM	4025	N	SER D 133	101.412	53.499	23.979	1.00 22.08	D
ATOM	4026	CA	SER D 133	100.622	52.307	24.251	1.00 21.07	D
	4027	СВ	SER D 133	99.405	52.637	25.119	1.00 21.95	D
ATOM			SER D 133	98.567	53.595	24.498	1.00 27.01	D
ATOM	4028	OG				22.908	1.00 21.27	ם
MOTA	4029	C	SER D 133	100.178	51.738			D
ATOM	4030	0	SER D 133	100.344	52.369	21.864	1.00 19.82	
ATOM	4031	N	GLU D 134	99.627	50.538	22.926	1.00 20.29	D
MOTA	4032	CA	GLU D 134	99.182	49.938	21.689	1.00 24.12	D
ATOM	4033	CB	GLU D 134	100.370	49.323	20.932	1.00 26.01	D
ATOM	4034	CG	GLU D 134	100.932	48.045	21.532	1.00 30.80	D
ATOM	4035	CD	GLU D 134	102.080	47.480	20.704	1.00 35.43	D
MOTA	4036		GLU D 134	102.273	46.243	20.702	1.00 36.93	D
			GLU D 134	102.793	48.278	20.057	1.00 37.66	D
ATOM	4037				48.882	21.955	1.00 22.81	D
MOTA	4038	C	GLU D 134	98.127			1.00 22.94	D
MOTA	4039	0	GLU D 134	97.968	48.416	23.081		
MOTA	4040	N	THR D 135	97.400	48.522	20.908	1.00 21.95	D
ATOM	4041	CA	THR D 135	96.361	47.519	21.009	1.00 20.78	Q
ATOM	4042	CB	THR D 135	95.368	47.625	19.843	1.00 20.82	D
ATOM	4043	OG	THR D 135	96.032	47.262	18.623	1.00 22.24	D
ATOM	4044	CG	THR D 135	94.833	49.046	19.721	1.00 18.01	D
MOTA		c	THR D 135	97.037	46.168	20.890	1.00 20.80	D
	4045		THR D 135	98.259	46.084	20.742	1.00 21.08	D
MOTA	4046	0					1.00 19.11	D
MOTA	4047	N	SBR D 136	96.234	45.116	20.972		
ATOM	4048	CA	SER D 136	96.728	43.764	20.790	1.00 16.93	D
ATOM	4049	CB	SER D 136	95.769	42.755	21.428	1.00 19.17	D
ATOM	4050	OG	SER D 136	95.656	42.951	22.831	1.00 23.01	D
MOTA	4051	C	SER D 136	96.665	43.635	19.267	1.00 15.30	D
ATOM	4052	o	SER D 136	96.325	44.592	18.580	1.00 13.19	D
ATOM	4053	N	PHE D 137	97.002	42.472	18.733	1.00 16.43	D
				96.896	42.267	17,294	1.00 16.20	D
MOTA	4054	CA					1.00 15.86	D
ATOM	4055	СВ		97.652	41.001	16.874	1.00 17.29	D
MOTA	4056	CG		99.138	41.146	16.879		
MOTA	4057		1 PHE D 137	99.792	41.775	15.823	1.00 20.23	D
ATOM	4058		2 PHB D 137	99.894	40.644	17.932	1.00 17.79	D
MOTA	4059		1 PHE D 137	101.187	41.900	15.815	1.00 21.20	D
ATOM	4060		2 PHE D 137	101.291	40.762	17.936	1.00 19.39	D
				101.935	41.392	16.874	1.00 19.70	D
MOTA	4061		PHE D 137	95.402	42.056	17.025	1.00 16.08	D
ATOM	4062			94.823	41.121	17.556	1.00 15.19	D
MOTA	4063		PHE D 137				1.00 19.23	D
MOTA	4064		LEU D 138	94.786	42.925	16.227		D
MOTA	4065	CA	LEU D 138	93.367	42.797	15.882	1.00 41.42	b

BEION	1000	CD.	LEU D 138	92.722	44.175	15.678	1.00 21.40	Ð
MOTA	4066	CB		92.452	45.087	16.881	1.00 22.42	D
ATOM	4067	CG	LEU D 138	91.889		.18.032	1.00 23.38	Ď
ATOM	4068		LEU D 138					
ATOM	4069		LEU D 138	93.732	45.764	17.301	1.00 28.68	D
MOTA	4070	C	TEO D 138	93.230	41.982	14.593	1.00 20.56	D
MOTA	4071	0	LEU D 138	93.919	42.244	13.615	1.00 22.27	D
MOTA	4072	N	SER D 139	92.326	41.013	14.586	1.00 20.44	D
MOTA	4073	CA	SER D 139	92.143	40.142	13.427	1.00 19.23	D
MOTA	4074	CB	SER D 139	91.222	38.986	13.788	1.00 19.74	D
MOTA	4075	OG	SER D 139	89.888	39.443	13.861	1.00 21.32	D
MOTA	4076	C	SER D 139	91.594	40.802	12.168	1.00 19.43	D,
MOTA	4077	0	SER D 139	91.028	41.893	12.210	1.00 19.49	D
ATOM	4078	N	LYS D 140	91.755	40.102	11.050	1.00 18.62	D
ATOM	4079	CA	LYS D 140	91.276	40.553	9.749	1.00 19.20	D
ATOM	4080	CB	LYS D 140	92.437	41.058	8.895	1.00 18.92	D
ATOM	4081	CG	LYS D 140	93.286	42.126	9.554	1.00 19.38	D
MOTA	4082	CD	LYS D 140	93.254	43.393	8.758	1.00 20.95	D
ATOM	4083	CE	LYS D 140	93.833	43.195	7.377	1.00 18.23	D
MOTA	4084	NZ	LYS D 140	93.743	44.457	6.617	1.00 20.40	D
		C	LYS D 140	90.660	39.339	9.068	1.00 19.16	D
MOTA	4085		LYS D 140	91.091	38.217	9.312	1.00 19.77	D
MOTA	4086	0			39.552	8.207	1.00 21.60	D
MOTA	4087	N	SER D 141	89.670			1.00 23.19	D
MOTA	4088	CA	SER D 141	89.030	38.438	7.507		D
ATOM	4089	CB	SER D 141	87.859	38.948	6.653	1.00 24.88	
MOTA	4090	OG	SER D 141	88.288	39.858	5.655	1.00 28.69	D
ATOM	4091	С	SER D 141	89.989	37.605	6.636	1.00 23.26	D
ATOM	4092	0	SER D 141	89.692	36.454	6.327	1.00 23.33	D
MOTA	4093	N	ASP D 142	91.137	38.159	6.251	1.00 21.38	D
ATOM	4094	CA	ASP D 142	92.075	37.387	5.429	1.00 22.54	D
ATOM	4095	CB	ASP D 142	92.834	38.303	4.466	1.00 25.84	D
ATOM	4096	CG	ASP D 142	93.943	39.064	5.143	1.00 29.78	D
MOTA	4097	OD1	ASP D 142	93.760	39.486	6.309	1.00 31.16	D
ATOM	4098	OD2	ASP D 142	94.997	39.246	4.500	1.00 34.64	D
MOTA	4099	c	ASP D 142	93.045	36.637	6.336	1.00 22.89	D
ATOM	4100	ō	ASP D 142	94.027	36.037	5.883	1.00 20.54	D
ATOM	4101	N	HIS D 143	92.753	36.700	7.632	1.00 21.06	D
ATOM.	4102	CA	HIS D 143	93.522	36.020	8.659	1.00 19.58	D
		CB	HIS D 143	93.628	34.534	8.317	1.00 19.03	D
ATOM	4103	CG	HIS D 143	92.295	33.892	8.104	1.00 23.00	D
ATOM	4104				33.108	7.104	1.00 24.78	D
MOTA	4105		HIS D 143	91.827		8.967	1.00 21.97	D
MOTA	4106		. HIS D 143	91.237	34.087		1.00 24.67	D
ATOM	4107		. HIS D 143	90.174	33.455	8.505		D
MOTA	4108		HIS D 143	90.504	32.853	7.375	1.00 24.72	
MOTA	4109	C	HIS D 143	94.878	36.602	8.986	1.00 20.11	D
ATOM	4110	0	HIS D 143	95.691	35.962	9.654	1.00 21.09	D
MOTA	4111	N	SER D 144	95.118	37.820	8.514	1.00 21.24	D
MOTA	4112	CA.	SER D 144	96.352	38.525	8.826	1.00 21.79	a
ATOM	4113	CB	SER D 144	96.834	39.353	7.627	1.00 20.33	D
MOTA	4114	OG	SER D 144	96.047	40.511	, 7.434	1.00 24.32	D
MOTA	4115	C	SER D 144	95.940	39.440	9.990	1.00 21.43	D
ATOM	4116	0	SER D 144	94.830	39.317	10.504	1.00 20.74	D
ATOM	4117	N	PHE D 145	96.809	40.352	10.412	1.00 21.56	D
ATOM	4118	CA	PHE D 145	96.463	41.235	11.523	1.00 22.54	D
MOTA	4119	СВ	PHE D 145	97.156	40.791	12.817	1.00 22.63	D
ATOM	4120	CG	PHE D 145	96.896	39.368	13.200	1.00 25.73	D
ATOM	4121		1 PHE D 145		38.329	12.562	1.00 26.67	D
	4122		2 PHE D 145		39.063	14.207	1.00 23.65	D
ATOM			1 PHE D 145		37.004	12.921	1.00 27.30	D
ATOM	4123		2 PHE D 145		37.746	14.572	1.00 25.43	D
ATOM	4124						1.00 24.90	D
MOTA	4125	CZ	PHE D 145		36.713	13.926 11.299	1.00 22.51	D
ATOM	4126	С	PHE D 145		42.687		1.00 23.97	Ď
MOTA	4127	0	PHE D 145			10.339		
MOTA	4128	N.	PHE D 146		43.540	12.198	1.00 20.96	D
MOTA	4129	CA			44.946	12.190	1.00 19.68	D
ATOM	4130	CB				11.439	1.00 17.70	D
ATOM	4131	CG	PHE D 146			12.159	1.00 15.76	D
MOTA	4132		1 PHE D 146			12.948	1.00 16.08	D
ATOM	4133	CD	2 PHE D 146	93.321	45.170	11.976	1.00 14.70	D
ATOM	4134		1 PHE D 146	92.961	47.442	13.543	1.00 13.47	D
ATOM	4135		2 PHE D 146		45.426	12,563	1.00 15.43	D
MOTA	4136				46.567	13.350	1.00 14.68	D
ATOM	4137		PHE D 146		45.335	13.654		D
ATOM	4138		PHE D 146				1.00 19.92	Œ
ATOM	4139		LYS D 14					ם

MOTA	4140	CA	LYS D 147	97.910	46.817	15.260	1.00 19.84	D
MOTA	4141	CB	LYS D 147	99.184	46.148	15.796	1.00 21.50	D
ATOM	4142	CG	LYS D 147	99.651	46.679	17.134	1.00 24.87	D
MOTA	4143	CD	LYS D 147	100.764	45.832	17.724	1.00 27.18	D
				100.220	44.515	18.253	1.00 31.41	D
ATOM	4144	CE	LYS D 147					
MOTA	4145	NZ	LYS D 147	101.086	43.984	19.341	1.00 32.97	D
MOTA	4146	С	LYS D 147	98.038	48.324	15.274	1.00 18.69	D
ATOM	4147	0	LYS D 147	98.603	48.914	14.352	1.00 20.14	D
ATOM	4148	N	ILE D 148	97.497	48.944	16.314	1.00 18.22	Q
ATOM	4149	CA	ILE D 148	97.530	50.387	16.446	1.00 18.25	D
MOTA	4150	CB	ILE D 148	96.092	50.942	16.548	1.00 20.80	D
MOTA	4151	CG2	ILE D 148	96.113	52.459	16.659	1.00 22.44	D
MOTA	4152	CG1	ILE D 148	95.308	50.533	15.292	1.00 23.89	D
MOTA	4153	CD1	ILE D 148	93.840	50.858	15.314	1.00 24.42	D
MOTA	4154	C	ILE D 148	98.369	50.816	17.646	1.00 19.71	D
			ILE D 148	98.213	50.294	18.757	1.00 17.77	D
MOTA	4155	0						
MOTA	4156	N	SER D 149	99.284	51.753	17.395	1.00 19.08	D
MOTA	4157	CA	SER D 149	100.173	52.278	18.424	1.00 18.19	D
MOTA	4158	CB	SER D 149	101.633	52.137	17.991	1.00 18.51	D
MOTA	4159	OG	SER D 149	102.518	52.492	19.040	1.00 19.49	D
ATOM	4160	C	SER D 149	99.839	53.744	18.646	1.00 18.14	D
						17.693	1.00 18.17	D
MOTA	4161	0	SER D 149	99.591	54.490			
MOTA	4162	N	TYR D 150	99.843	54.155	19.905	1.00 16.95	D
MOTA	4163	CA	TYR D 150	99.503	55.524	20.261	1.00 16.12	D
MOTA	4164	CB	TYR D 150	98.310	55.524	21.213	1.00 15.57	D
MOTA	4165	CG	TYR D 150	97.116	54.750	20.701	1.00 16.81	D
	4166		TYR D 150	96.291	55.276	19.709	1.00 14.33	D
ATOM								D
ATOM	4167		TYR D 150	95.197	54.554	19.222	1.00 17.50	
MOTA	4168	CD2	TYR D 150	96.819	53.486	21.199	1.00 15.90	D
ATOM	4169	CE2	TYR D 150	95.731	52.760	20.719	1.00 18.41	D
ATOM	4170	CZ	TYR D 150	94.928	53.297	19.732	1.00 16.27	D
ATOM	4171	OH	TYR D 150	93.868	52.574	19.244	1.00 20.03	D
	4172	C	TYR D 150	100.650	56.266	20.922	1.00 16.35	D
ATOM					55.690		1.00 16.95	D
ATOM	4173	0	TYR D 150	101.438		21.669		
ATOM	4174	N	LEU D 151	100.732	57.558	20.643	1.00 16.64	D
ATOM	4175	CA	LEU D 151	101.760	58.396	21.227	1.00 16.50	D
MOTA	4176	CB	LEU D 151	102.849	58.705	20.203	1.00 15.48	D
ATOM	4177	CG	LEU D 151	103.806	59.825	20.639	1.00 17.55	D
			LEU D 151	104.641	59.374	21.834	1.00 16.60	D
MOTA	4178						1.00 16.11	Đ
MOTA	4179	-	LEU D 151	104.702	60.213	19.476		
ATOM	4180	С	LEU D 151	101.140	59.701	21.693	1.00 17.56	D
MOTA	4181	0	LEU D 151	100.577	60.440	20.888	1.00 17.18	D
MOTA	4182	N	THR D 152	101.233	59.997	22.983	1.00 16.14	D
ATOM	4183	CA	THR D 152	100.690	61.259	23.448	1.00 19.47	D
	4184	CB	THR D 152	100.359	61.248	24.966	1.00 21.24	D
MOTA					60.871	25.725	1.00 25.03	D
MOTA	4185		THR D 152	101.517				
MOTA	4186	CG2		99.214	60.281	25.247	1.00 20.79	D
ATOM	4187	C	THR D 152	101.717	62.345	23.151	1.00 19.82	D
MOTA	4188	0	THR D 152	102.921	62.113	23.218	1.00 21.31	D
ATOM	4189	N	LEU D 153	101.241	63.523	22.781	1.00 20.76	D
MOTA	4190	CA	LEU D 153	102.143	64.617	22.488	1.00 24.15	D
		CB	LEU D 153	102.760	64.450	21.089	1.00 25.45	D
MOTA	4191			101.959	64.575	19.785	1.00 27.17	D
MOTA	4192	CG	LEU D 153					
MOTA	4193		LEU D 153	100.520	64.101	19.986	1.00 27.83	D
MOTA	4194	CD2	LEU D 153	101.982	66.015	19.319	1.00 27.38	D
MOTA	4195	С	LEU D 153	101.440	65.952	22.601	1.00 25.73	D
ATOM	4196	0	LEU D 153	100.208	66.028	22.681	1.00 26.55	D
		N	LEU D 154	102.251	67.000	22.640	1.00 26.77	D
ATOM	4197					22.734	1.00 26.34	ם
MOTA	4198	CA	LEU D 154	101.781	68.369			
MOTA	4199	CB	LEU D 154	102.298	69.027	24.019	1.00 25.08	D
MOTA	4200	CG	LEU D 154	101.877	70.478	24.288	1.00 26.28	D
ATOM	4201	CD1	LEU D 154	100.377	70.531	24.570	1.00 24.44	D
ATOM	4202		LEU D 154	102.667	71.031	25.477	1.00 23.08	Ø
ATOM	4203	C	LEU D 154	102.374	69.063	21.522	1.00 28.41	D
			LEU D 154	103.577	69.327	21.468	1.00 27.19	D
MOTA	4204	0						
ATOM	4205	N	PRO D 155	101.534	69.351	20.523	1.00 30.32	D
MOTA	4206	æ	PRO D 155	100.109	68.979	20.453	1.00 30.25	D
MOTA	4207	CA	PRO D 155	101.965	70.014	19.294	1.00 31.71	D
MOTA	4208	CB	PRO D 155	100.667	70.160	18.510	1.00 31.92	D
MOTA	4209	CG	PRO D 155	99.861	68.968	18.963	1.00 31.51	D
		C	PRO D 155	102.663	71.354	19.508	1.00 35.12	D
MOTA	4210	-				20.112	1.00 35.64	D
MOTA	4211	0	PRO D 155	102.110	72.275			
MOTA	4212		SER D 156	103.893	71.436	19.014	1.00 39.00	D
MOTA	4213	CA	SER D 156	104.706	72.643	19.083	1.00 42.94	D

4214 CB SER D 156 MOTA 105.819 72.492 20.121 1.00 43.03 MOTA 4215 OG SER D 156 105.288 72.385 21.430 1.00 45.30 ATOM 4216 C SER D 156 105.311 72.763 17.694 1.00 46.03 104.875 72.084 16.770 1.00 47.06 ATOM 4217 O SER D 156 106.316 73.609 17.534 1.00 49.61 ATOM 4218 N ALA D 157 ATOM 4219 CA ALA D 157 106.931 73.756 16.222 1.00 51.03 ATOM 4220 CB ALA D 157 106.977 75.231 15.828 1.00 51.20 ALA D 157 108.334 73.163 16.195 1.00 51.50 ATOM 4221 C 108.985 73.147 15.150 1.00 52.20 ATOM 4222 O ALA D 157 108.797 72.669 17.339 1.00 52.37 ATOM 4223 N GLU D 158 110.141 72.103 17.411 1.00 53.43 MOTA 4224 CA GLU D 158 GLU D 158 110.946 72.785 18.524 1.00 57.17 MOTA 4225 CB 110.401 72.570 19.934 1.00 61.50 ATOM 4226 CG GLU D 158 MOTA 4227 CD GLU D 158 109.278 73.529 20.291 1.00 63.75 108.757 73.431 21.425 1.00 63.56 ATOM 4228 OE1 GLU D 158 108.922 74.381 19.445 1.00 65.17 4229 OB2 GLU D 158 MOTA ATOM 4230 C GLU D 158 110.190 70.592 17.614 1.00 51.03 D 4231 0 GLU D 158 111.103 70.084 18.265 1.00 51.07 D ATOM 109.219 69.876 17.057 1.00 47.47 GLU D 159 ATOM 4232 N 109.185 68.425 17.193 1.00 46.22 4233 CA GLU D 159 ATOM 108.337 68.013 18.406 1.00 47.11 ATOM 4234 СВ GLU D 159 D GLU D 159 109.127 67.692 19.671 1.00 48.53 ATOM 4235 CG 108.268 67.042 20.751 1.00 50.37 ATOM 4236 CD GLU D 159 107.319 67.694 21.238 1.00 50.39 OE1 GLU D 159 ATOM 4237 108.537 65.873 21.112 1.00 50.03 D 4238 OE2 GLU D 159 MOTA GLU D 159 108.641 67.714 15.960 1.00 43.84 D MOTA 4239 C 107.515 67.974 15.535 1.00 44.12 4240 GLU D 159 MOTA 0 109.443 66.825 15.380 1.00 39.56 SER D 160 ATOM 4241 N 108.993 66.054 14.229 1.00 37.29 MOTA 4242 CA **SER D 160** SER D 160 109.971 66.172 13.055 1.00 37.41 ATOM 4243 CB 4244 OG SER D 160 111.070 65.298 13.206 1.00 41.72 ATOM 108.933 64.615 14.734 1.00 35.08 SER D 160 ATOM 4245 C 109.754 64.207 15.557 1.00 33.66 4246 O SER D 160 ATOM MOTA 4247 N TYR D 161 107.961 63.846 14.260 1.00 32.11 4248 CA TYR D 161 107.828 62.478 14.728 1.00 29.69 ATOM 1.00 29.62 TYR D 161 106.550 62.315 15.547 ATOM 4249 CB 106.347 63.349 16.620 1.00 29.33 ATOM 4250 CG TYR D 161 CD1 TYR D 161 105.761 64.577 16.327 1.00 31.31 D MOTA 4251 CE1 TYR D 161 105.513 65.515 17.329 1.00 32.70 D ATOM 4252 106.695 63.085 17.937 1.00 30.13 CD2 TYR D 161 MOTA 4253 106.457 64.013 18.947 1.00 30.43 105.863 65.223 18.638 1.00 31.92 ATOM 4254 CE2 TYR D 161 4255 CZ TYR D 161 D ATOM 105.592 66.128 19.643 1.00 35.12 ATOM 4256 OH TYR D 161 TYR D 161 107.820 61.441 13.627 1.00 29.60 4257 С MOTA 1.00 29.45 TYR D 161 107.493 61.728 12.473 MOTA 4258 0 108.172 60.221 14.005 1.00 29.35 D 4259 ASP D 162 ATOM N CA ASP D 162 108.201 59.109 13.075 1.00 30.15 D ATOM 4260 109.618 58.863 12.548 1.00 34.90 CB ASP D 162 4261 ATOM 110.154 60.016 11.733 1.00 37.70 D MOTA 4262 CG ASP D 162 OD1 ASP D 162 109.669 60.218 10.597 1.00 40.13 D MOTA 4263 OD2 ASP D 162 111.061 60.716 12.235 1.00 38.68 ATOM 4264 C ASP D 162 107.759 57.851 13.784 1.00 29.84 MOTA 4265 1.00 26.72 108.010 57.672 14.978 D 4266 0 ASP D 162 MOTA CYS D 163 107.088 56.984 13.039 1.00 29.31 D MOTA 4267 N 106.684 55.700 13.569 1.00 29.59 4268 CA CYS D 163 D MOTA CYS D 163 107.689 54.769 12.902 1.00 28.04 ATOM 4269 C 107.822 54.772 11.685 1.00 26.22 D 4270 0 CYS D 163 ATOM MOTA 4271 CB CYS D 163 105.265 55.326 13.134 1.00 29.11 D SG CYS D 163 104.703 53.760 13.878 1.00 34.32 D MOTA 4272 1.00 29.03 LYS D 164 108.417 54.001 13.699 N ATOM 4273 109.404 53.072 13.161 1.00 29.67 CA LYS D 164 ATOM 4274 110.730 53.238 13.911 1.00 32.54 ATOM 4275 CB LYS D 164 D LYS D 164 111.874 52.352 13.416 1.00 34.76 4276 CG D MOTA 113.109 52.528 14.297 LYS D 164 1.00 34.79 CD ATOM 4277 1.00 38.29 ATOM 4278 CE LYS D 164 114.254 51.630 13.850 14.775 4279 LYS D 164 115.425 51.702 1.00 36.58 MOTA NZ 4280 C LYS D 164 108.863 51.651 13.322 1.00 28.94 D ATOM 1.00 29.32 LYS D 164 108.642 51.189 14.443 ATOM 4281 0 VAL D 165 108.632 50.974 12.197 1.00 27.33 ATOM 4282 N VAL D 165 12.212 1.00 26.58 4283 CA 108.100 49.618 ATOM 1.00 27.12 VAL D 165 106.797 49.516 11.359 ATOM 4284 CB CG1 VAL D 165 106.199 48.122 11.462 1.00 25.56 ATOM 4285 1.00 27.97 CG2 VAL D 165 105.787 50.544 11.827 ATOM 4286 109.113 48.600 11.690 1.00 26.91 VAL D 165 ATOM 4287 С

ATOM	4288	0	VAL D	165	109.621	48.720	10.583	1.00 25.56	D
MOTA	4289	N	GLU D	166	109.414	47.606	12.513	1.00 28.75	D
ATOM	4290	CA	GLU D		110.338	46.544	12.139	1.00 30.67	D
		CB	GLU D		111.445	46.410	13.194	1.00 33.57	מ
MOTA	4291						13.142	1.00 41.68	Ď
ATOM	4292	CG	GLU D		112.452	47.565			
MOTA	4293	CD	GLU D		113.506	47.526	14.244	1.00 46.12	D
MOTA	4294	OB1	GLU D	166	114.482	48.304	14.146	1.00 49.01	D
MOTA	4295	OE2	GLU D	166	113.363	46.736	15.206	1.00 49.40	D
ATOM	4296	C	GLU D	166	109.543	45.243	12.008	1.00 30.18	D
ATOM	4297	ō	GLU D		108.737	44.900	12.878	1.00 28.51	D
						44.535	10.907	1.00 29.48	D
MOTA	4298	N	HIS D		109.759				
ATOM	4299	CA	HIS D		109.056	43.281	10.648	1.00 30.29	D
ATOM	4300	CB	HIS D	167	107.686	43.569	10.025	1.00 29.56	D
ATOM	4301	CG	HIS D	167	106.808	42.363	9.903	1.00 30.02	D
MOTA	4302	CD2	HIS D	167	106.562	41.541	8.856	1.00 29.91	D
ATOM	4303		HIS D		106.068	41.871	10.957	1.00 31.27	D
			HIS D		105.404	40.798	10.564	1.00 28.43	D
ATOM	4304							1.00 28.97	D
MOTA	4305		HIS D		105.687	40.576	9.293		
MOTA	4306	C	HIS D	167	109.886	42.440	9.684	1.00 30.36	D
ATOM	4307	0	HIS D	167	110.607	42.976	8.842	1.00 30.66	D
MOTA	4308	N	TRP D	168	109.775	41.122	9.801	1.00 31.13	D
ATOM	4309	CA	TRP D	168	110.521	40.219	8.930	1.00 32.08	D
MOTA	4310	СВ	TRP D		110.270	38.765	9.336	1.00 28.28	D
						38.475	10.739	1.00 26.36	D
MOTA	4311	CG		168	110.665				
MOTA	4312	CD2	TRP D	168	110.031	37.556	11.635	1.00 25.51	D
MOTA	4313	CE2	TRP D	168	110.759	37.578	12.842	1.00 26.35	D
ATOM	4314	CE3	TRP D	168	108.916	36.715	11.534	1.00 24.88	D
MOTA	4315		TRP D	168	111.721	39.004	11.416	1.00 27.27	D
ATOM	4316		TRP D		111.786	38.471	12.682	1.00 28.25	D
					110.412	36.791	13.943	1.00 27.00	D
MOTA	4317	CZ2							D
ATOM	4318	CZ3			108.568	35,932	12.628	1.00 25.90	
MOTA	4319	CH2	TRP D	168	109.315	35.976	13.817	1.00 26.65	D
ATOM ·	4320	С	TRP D	168	110.180	40.403	7.452	1.00 33.22	D
MOTA	4321	0	TRP D	168	111.011	40.139	6.582	1.00 33.90	Ø
ATOM	4322	N	GLY D	169	108.959	40.853	7.174	1.00 34.75	D
ATOM	4323	CA	GLY D		108.533	41.060	5.797	1.00 36.14	D
			GLY D		109.056	42.359	5.215	1.00 37.80	D
MOTA	4324	C					4.139	1.00 36.95	D
ATOM	4325	0	GLY D		108.635	42.796			
MOTA	4326	N	TEO D	170	109.979	42.981	5.938	1.00 38.89	D
ATOM	4327	CA	LEU D	170	110.578	44.234	5.509	1.00 40.79	D
ATOM	4328	CB	LEU D	170	110.212	45.356	6.480	1.00 39.77	D
ATOM	4329	CG	TEO D	170	108.745	45.765	6.581	1.00 39.57	D
ATOM	4330		LEU D		108.592	46.809	7.671	1.00 38.10	D
			LEU D		108.267	46.308	5.243	1.00 39.58	D
MOTA	4331						5.465	1.00 42.12	D
MOTA	4332	С	LEO D		112.092	44.085			
ATOM	4333	0	LEU D		112.688	43.506	6.370	1.00 41.54	D
ATOM	4334	N	ASP D	171	112.706	44.613	4.411	1.00 45.36	D
MOTA	4335	CA	ASP D	171	114.158	44.559	4.252	1.00 48.35	D
MOTA	4336	CB	ASP D	171	114.539	44.947	2.820	1.00 50.69	D
MOTA	4337	CG	ASP D	171	113.467	45.775	2.137	1.00 52.75	D
			L ASP I		113.076	46.827	2.689	1.00 54.19	D
ATOM	4338						1.046	1.00 54.32	D
ATOM	4339		2 ASP I		113.012	45.372			
MOTA	4340	С	ASP I		114.849	45.485	5.255	1.00 48.43	D
MOTA	4341	0	asp I	171	115.816	45.090	5.910	1.00 48.29	D
ATOM	4342	N	LYS I	172	114.348	46.715	5.364	1.00 48.92	D
ATOM	4343	CA	LYS I	172	114.883	47.707	6.299	1.00 49.86	D
ATOM	4344	CB	LYS I		115.502	48.898	5.552	1.00 51.58	D
		CG	LYS I		116.667	48.566	4.637	1.00 55.86	D
MOTA	4345					47.963	3.316	1.00 58.23	D
MOTA	4346	CD	LYS I		116.203				
MOTA	4347	CE	LYS I		115.408	48.966	2.493	1.00 59.62	D
ATOM	4348	NZ	LYS I	172	114.946	48.368	1.211	1.00 59.53	D
MOTA	4349	С	LYS I	172	113.734	48.224	7.165	1.00 48.46	D
ATOM	4350	0	LYS I	172	112.564	48.026	6.833	1.00 48.43	D
ATOM	4351	N		173	114.050	48.885	8.291	1.00 46.54	D
	4352	CD		173	115.355	49.048	8.954	1.00 46.03	D
ATOM						49.400	9.137		D
MOTA	4353	CA		173	112.974				D
ATOM	4354	СВ		173	113.722	50.029			
MOTA	4355			D 173	114.950	49.197			D
MOTA	4356	С	PRO 1	D 173	112.180				D
ATOM	4357		PRO 1	D 173	112.746	51.197	7.570	1.00 43.42	D
ATOM	4358			D 174	110.869			1.00 41.53	D
MOTA	4359			D 174	110.023				D
	4360			D 174	108.675			1.00 40.30	D
ATOM									D
MOTA	4361	ÇG	neo :	D 174	107.900	21.463	0.505	2.00 20.33	

ATOM	4362	CD1	LEU I	D	174	106.637	50.397	6.151	1.00 42.25	D
ATOM	4363		LEU I			107.568	52.698	6.448	1.00 42.67	D
MOTA	4364	С	LEU 1	D	174	109.845	52.586	8.753	1.00 39.80	D
MOTA	4365	0	LEU !	D	174	109.645	52.420	9.955	1.00 39.99	D
MOTA	4366	N	LEU 1			109.947	53.792	8.200	1.00 38.49	D
MOTA	4367	CA	TEO 1			109.787	55.016	8.983	1.00 38.04	D
ATOM	4368	CB	TEO 1			111.095	55.812	9.045	1.00 38.62	D
ATOM	4369	CG	PEO ;			112.127	55.442	10.113	1.00 38.70	D
MOTA	4370		TEO :			111.518	55.648	11.489	1.00 39.24	D D
ATOM	4371		LEU !			112.577	54.001	9.936 8.372	1.00 40.07 1.00 37.31	D
ATOM	4372	C 0	LEU :			108.712 108.885	55.892 56.432	7.282	1.00 37.51	ם
ATOM ATOM	4373 4374	N	LYS			107.599	56.033	9.076	1.00 35.14	Ď
ATOM	4375	CA	LYS			106.511	56.850	8.577	1.00 34.26	D
ATOM	4376	СВ	LYS			105.175	56.124	8.768	1.00 33.88	D
ATOM	4377	CG	LYS			104.204	56.325	7.620	1.00 36.72	מ
ATOM	4378	CD	LYS :	D	176	104.829	55.887	6.295	1.00 37.68	D
MOTA	4379	CE	LYS :	D	176	103.820	55.913	5.155	1.00 39.32	D
ATOM	4380	NZ	LYS	D	176	103.195	57.254	4.974	1.00 40.75	D
MOTA	4381	C	LYS			106.523	58.166	9.335	1.00 32.22	D
MOTA	4382	0	LYS			106.272	58.204	10.537	1.00 32.35	D
ATOM	4383	N	HIS			106.825	59.243	8.625	1.00 29.85	D D
ATOM	4384	CA	HIS			106.897	60.563	9.229	1.00 29.87	D
ATOM	4385	CB	HIS			107.836	61.456 62.830	8.411 8.979	1.00 30.84 1.00 31.41	D
ATOM	4386	CG	HIS			108.014 107.607	64.042	8.529	1.00 32.01	D
MOTA MOTA	4387 4388		HIS			108.695	63.067	10.155	1.00 32.16	D
ATOM	4389		HIS			108.704	64.365	10.402	1.00 30.49	D
ATOM	4390		HIS			108.051	64.979	9.431	1.00 31.08	D
ATOM	4391	C	HIS			105.532	61.228	9.332	1.00 29.28	D
ATOM	4392	0	HIS	D	177	104.709	61.121	8.429	1.00 27.97	D
ATOM	4393	N	TRP	D	178	105.295	61.922	10.439	1.00 29.05	D
MOTA	4394	CA	TRP		178	104.031	62.617	10.619	1.00 29.38	D
ATOM	4395	CB	TRP			103.518	62.464	12.048	1.00 26.73	D
MOTA	4396	CG	TRP			102.205	63.165	12.243	1.00 27.32 1.00 24.87	D D
ATOM	4397		TRP		178 178	101.939 100.580	64.262 64.608	13.122 12.959	1.00 26.97	D
ATOM	4398 4399	CE2				102.714	64.986	14.033	1.00 26.15	D
ATOM ATOM	4400		TRP			101.028	62.898	11.599	1.00 26.41	ם D
ATOM	4401	NE1			178	100.050	63.759	12.023	1.00 25.31	D
ATOM	4402	CZ2				99.980	65.649	13.675	1.00 25.60	D
ATOM	4403	CZ3	TRP	D	178	102.118	66.021	14.746	1.00 27.98	D
ATOM	4404		TRP			100.763	66.340	14.562	1.00 27.02	D
MOTA	4405	C	TRP			104.185	64.100	10.294	1.00 30.33	D
MOTA	4406	0	TRP			104.756 103.745	64.824 64.512	11.143 9.193	1.00 29.85 1.00 32.23	D D
ATOM	4407	OXT CB	TRP		3	113.641	35.776	8.019	1.00 59.19	E
ATOM ATOM	4408 4409	OG	SER		3	112.349	35.748	8.608	1.00 59.65	E
ATOM	4410	C	SER		3	114.352	33.977	9.601	1.00 57.92	E
MOTA	4411	ō	SER		3	114.571	32.945	8.970	1.00 57.45	E
ATOM	4412	N	SER	E	3	116.055	35.305	8.352	1.00 59.31	E
ATOM	4413	CA	SER	E	3	114.719	35.342	9.020	1.00 58.85	E
MOTA	4414	N	PRO	B	4	113.799	33.958	10.824	1.00 56.65	E
MOTA	4415	CD	PRO		4	113.679	35.092	11.759	1.00 56.20	E
MOTA	4416	CA	PRO		4	113.403	32.704	11.472	1.00 55.50	E
MOTA	4417	CB	PRO		4	113.362	33.086	12.946	1.00 56.49	E
MOTA	4418	CG	PRO		4	112.870 112.046	34.493 32.217	12.893 10.957	1.00 56.56 1.00 53.68	E
MOTA MOTA	4419 4420	C O	PRO PRO		4	111.168	33.024	10.648	1.00 54.06	E
ATOM	4421	N	GLU		5	111.875	30.903	10.855	1.00 51.52	E
MOTA	4422	CA	GLU			110.610	30.360	10.373	1.00 49.69	E
ATOM	4423	CB	GLU			110.831	29.007	9.676	1.00 53.42	E
MOTA	4424	CG	GLU			111.305	27.867	10.561	1.00 57.99	E
MOTA	4425	CD	GLU	E	5	111.671	26.626	9.758	1.00 60.86	E
ATOM	4426		GLU			110.857	26.196	8.908	1.00 62.41	E
MOTA	4427		GLU			112.772	26.077	9.979	1.00 63.42	E
MOTA	4428	C	GLU			109.619	30.231	11.525	1.00 45.48 1.00 46.07	e
MOTA	4429	0	GLU			109.919	29.644 30.800	12.564 11.337	1.00 40.87	E
MOTA MOTA	4430 4431	N CA	asp asp			108.436 107.403	30.782	12.363	1.00 36.20	E
ATOM	4432	CB	ASP			106.911	32.214	12.617	1.00 35.53	E
ATOM	4433	CG	ASP			105.995	32.323	13.827	1.00 33.60	B
ATOM	4434		LASP			105.185	33.268	13.864	1.00 34.88	E
MOTA	4435	OD:	asp	E	6	106.089	31.487	14.748	1.00 33.84	E

MOTA	4436	C	ASP	B	6	106.229	29.915	11.938	1.00 33.07	B
ATOM	4437	0	ASP	B	6	105.882	29.867	10.762	1.00 32.95	E
ATOM	4438	N	PHE		7	105.632	29.228	12.906	1.00 31.08	B
ATOM	4439	CA	PHE		7	104.466	28.380	12.669	1.00 29.18	B
ATOM	4440	CB	PHE		7	104.760	26.950	13.116	1.00 31.11	B
MOTA	4441	CG	PHE		7	105.833	26.278	12.305	1.00 31.97	E
MOTA	4442			E	7	105.544	25.745	11.053	1.00 31.67	E
MOTA	4443	CD2	PHE	B	7	107.141	26.200	12.782	1.00 32.49	E
ATOM	4444	CE1	PHE	E	7	106.546	25.141	10.282	1.00 33.41	E
ATOM	4445	CE2	PHE	В	7	108.148	25.602	12.023	1.00 32.29	B
MOTA	4446	CZ	PHE		7	107.850	25.071	10.770	1.00 31.62	E
ATOM	4447	c	PHE		7	103.345	28.994	13.504	1.00 27.19	E
			PHE							E
MOTA	4448	0			7	103.483	29.151	14.715	1.00 25.77	
MOTA	4449	N		E	8	102.238	29.340	12.855	1.00 25.52	E
MOTA	4450	CA	VAL	E	8	101.127	29.998	13.538	1.00 23.97	E
MOTA	4451	CB	VAL	B	8	100.903	31.411	12.949	1.00 22.51	E
MOTA	4452	CG1	VAL	E	8	99.789	32.130	13.703	1.00 20.58	E
ATOM	4453	CG2	VAL	E	8	102.205	32.211	13.002	1,00 22.51	E
ATOM	4454	C	VAL		8	99.785	29.275	13.510	1.00 24.21	E
ATOM	4455	ō	VAL		8	99.369	28.736	12.485	1.00 25.26	E
ATOM	4456	N	TYR		9	99.096	29.288	14.643	1.00 23.98	E
ATOM	4457	CA	TYR		9	97.786	28.663	14.724	1.00 23.53	E
MOTA	4458	CB	TYR	E	9	97.796	27.505	15.718	1.00 24.07	B
ATOM	4459	CG	TYR	E	9	96.562	26.640	15.627	1.00 25.27	E
ATOM	4460	CD1	TYR	E	9	96.570	25.460	14.889	1.00 27.68	E
ATOM	4461	CEL	TYR		9	95.435	24.658	14.801	1.00 27.67	E
ATOM	4462	CD2	TYR		9	95.384	27.002	16.272	1.00 24.82	E
ATOM	4463	CE2	TYR		9	94.245	26.211	16.191	1.00 25.29	E
ATOM	4464	CZ	TYR		9	94.277	25.040	15.458	1.00 26.82	B
MOTA	4465	OH	TYR		9	93.163	24.240	15.403	1.00 27.65	B
MOTA	4466	C	TYR	E	9	96.775	29.707	15.179	1.00 23.14	B
MOTA	4467	0	TYR	E	9	97.037	30.476	16.106	1.00 23.66	e
ATOM	4468	N	GLN	E	10	95.622	29.739	14.523	1.00 21.64	E
MOTA	4469	CA	GLN	R	10	94.582	30.686	14.892	1.00 21.14	E
ATOM	4470	CB	GLN		10	94.438	31.793	13.843	1.00 20.35	E
		CG	GLN		10	95.677	32.598	13.529	1.00 19.58	B
ATOM	4471									B
ATOM	4472	CD	GLN		10	95.410	33.655	12.461	1.00 18.44	
ATOM	4473		GLN		10	94.498	34.474	12.593	1.00 19.00	B
MOTA	4474	NE2	GLN	Е	10	96.206	33.640	11.400	1.00 18.89	E
MOTA	4475	С	GLN	E	10	93.232	29.997	15.006	1.00 19.74	E
ATOM	4476	0	GLN	E	10	92.904	29.113	14.223	1.00 21.71	E
ATOM	4477	N	PHE	B	11	92.450	30.408	15.991	1.00 19.13	E
ATOM	4478	CA	PHE		11	91.108	29.887	16.145	1.00 16.86	E
MOTA	4479	СВ	PHE		11	90.981	28.881	17.271	1.00 16.74	E
ATOM	4480	CG	PHE		11	89.562	28.466	17.517	1.00 18.71	E
							27.615		1.00 21.10	E
MOTA	4481		PHE		11	88.910		16.626		
ATOM.	4482		PHE		11	88.849	28.985	18.595	1.00 18.11	E
MOTA	4483		PHE		11	87.559	27.290	16.807	1.00 22.40	E
MOTA	4484	CE2	PHE	Ε	11	87.499	28.671	18.789	1.00 15.75	E
ATOM	4485	CZ	PHE	E	11	86.854	27.826	17.898	1.00 21.25	E
MOTA	4486	C	PHE	E	11	90.218	31.069	16.451	1.00 17.10	B
MOTA	4487	0	PHE	E	11	90.461	31.819	17.406	1.00 13.97	E
ATOM	4488	N	LYS		12	89.197	31.241	15.622	1.00 16.07	E
ATOM	4489	CA	LYS		12	88.266	32.338	15.789	1.00 16.96	E
						88.308	33.246	14.564	1.00 17.05	8
MOTA	4490	CB	LYS		12					
ATOM	4491	CG	LYS		12	89.703	33.748	14.200	1.00 17.57	E
MOTA	4492	æ	LYS	E	12	89.663	34.535	12.888	1.00 18.92	R
MOTA	4493	CE	LYS	E	12	91.018	35.136	12.532	1.00 17.07	B
MOTA	4494	NZ	LYS	B	12	90.920	36.063	11.362	1.00 14.26	E
MOTA	4495	C	LYS	E	12	86.856	31.803	15.987	1.00 17.87	. В
ATOM	4496	0	LYS	B	12	86.354	31.039	15.165	1.00 16.82	B
MOTA	4497	N	GLY		13	86.235	32.195	17.098	1.00 18.19	B
MOTA	4498	CA	GLY		13	84.875	31.776	17.391	1.00 19.62	8
ATOM							32.939	17.010	1.00 19.93	E
	4499	C	GLY		13	83.991				
MOTA	4500	0	GLY		13	83.539	33.695	17.868	1.00 21.65	E
ATOM	4501	N	MET		14	83.728	33.070	15.715	1.00 19.89	B
MOTA	4502	CA	MET	E	14	82.947	34.184	15.197	1.00 20.54	E
MOTA	4503	CB	MET	E	14	83.430	34.490	13.785	1.00 21.02	E
ATOM	4504	CG	MET	E	14	84.937	34.657	13.751	1.00 23.04	E
ATOM	4505	SD	MET		14	85.587	35.218	12.190	1.00 25.32	E
ATOM	4506	CB	MET		14	85.218	36.938	12.284	1.00 20.32	E
ATOM	4507	C	MET		14	81.429	34.078	15.219	1.00 20.83	E
MOTA	4508		MET			80.859	32.999	15.101	1.00 20.77	E
		0			14					E
MOTA	4509	N	CYS	, E	15	80.789	35.232	15.377	1.00 20.66	25

3.000	4510	~	m/o 1		_	70 272	35.336	15.418	1.00 22.09	B
ATOM	4510	CA	CYS I		.5	79.332				
ATOM	4511	C	CYS I		.5	78.882	36.495	14.524	1.00 21.39	B
MOTA	4512	0	CXS 1	3	.5	79.393	37.614	14.644	1.00 19.38	E
ATOM	4513	CB	CYS 1	8 1	.5	78.841	35.616	16.848	1.00 22.10	B
ATOM	4514	SG	CYS I	B 1	.5	78.970	34.281	18.094	1.00 26.75	B
ATOM	4515	N	TYR I	B 1	.6	77.931	36.229	13.633	1.00 20.94	B
ATOM	4516	CA	TYR		.6	77.408	37.270	12.752	1.00 21.23	B
	4517	СВ	TYR		.6	77.548	36.858	11.287	1.00 18.37	B
MOTA										E
MOTA	4518	CG	TYR I		.6	78.972	36.574	10.876	1.00 19.23	
MOTA	4519	CD1	TYR !	B 1	.6	79.576	35.354	11.178	1.00 18.71	E
ATOM	4520	CE1	TYR I	B 1	.6	80.875	35.084	10.789	1.00 18.69	E
ATOM	4521	CD2	TYR I	E 1	L 6	79.715	37.524	10.178	1.00 20.25	B
ATOM	4522	CE2	TYR I	B 1	L 6	81.022	37.270	9.785	1.00 17.18	E
ATOM	4523	CZ	TYR		16	81.595	36.047	10.088	1.00 21.03	E
		OH	TYR		16	82.872	35.775	9.662	1.00 22.99	E
ATOM	4524									E
ATOM	4525	С	TYR :		L6	75.938	37.543	13.085	1.00 22.17	
ATOM	4526	0	TYR :		16	75.132	36.612	13.199	1.00 21.71	B
ATOM	4527	N	PHE :	E 1	17	75.607	38.825	13.247	1.00 23.05	E
ATOM	4528	CA	PHE :	E 1	L 7	74.254	39.263	13.591	1.00 23.67	E
MOTA	4529	CB	PHE :	B 3	L7	74.261	39.988	14.942	1.00 22.49	E
ATOM	4530	CG	PHE :	E 3	17	74.813	39.172	16.084	1.00 25.10	B
ATOM	4531		PHE		17	74.007	38.270	16.772	1.00 24.22	B
	4532	CD2			 L7	76.140	39.318	16.482	1.00 24.67	E
ATOM									1.00 24.68	E
MOTA	4533		PHE :		L7	74.516	37.526	17.844		
MOTA	4534	CE2	PHE		L7	76.656	38.579	17.548	1.00 24.45	E
MOTA	4535	CZ	PHE	E :	L7	75.843	37.684	18.228	1.00 24.13	B
MOTA	4536	C	PHE	E :	L7	73.673	40.223	12.549	1.00 25.10	B
MOTA	4537	0	PHE	B :	17	74.390	41.034	11.971	1.00 24.65	E
ATOM	4538	N	THR		18	72.365	40.122	12.333	1.00 27.15	R
ATOM	4539	CA	THR		18	71.638	40.983	11.405	1.00 29.69	B
		CB	THR		18	71.609	40.397	9.978	1.00 29.46	B
MOTA	4540								1.00 32.31	E
ATOM	4541		THR		18	72.949	40.252	9.500		
MOTA	4542	CG2	THR		18	70.863	41.321	9.032	1.00 28.09	E
MOTA	4543	C	THR	B :	18	70.217	41.080	11.950	1.00 31.56	E
ATOM	4544	0	THR	E :	18	69.638	40.071	12.355	1.00 32.09	E
ATOM	4545	N	ASN	E :	19	69.661	42.290	11.969	1.00 33.38	E
ATOM	4546	CA	ASN		19	68.316	42.495	12.497	1.00 35.02	E
	4547	СВ	ASN		19	67.279	41.755	11.647	1.00 37.99	E
ATOM						66.779	42.587	10.489	1.00 42.21	E
MOTA	4548	CG	ASN		19				1.00 47.70	E
MOTA	4549		ASN		19	66.271	43.695	10.687		
ATOM	4550	ND2	ASN	B :	19	66.910	42.063	9.273	1.00 43.13	E
ATOM	4551	C	asn	E :	19	68.264	41.977	13.924	1.00 34.10	E
ATOM	4552	0	asn	E	19	67.487	41.077	14.233	1.00 34.27	E
ATOM	4553	N	GLY	E	20	69.088	42.553	14.795	1.00 33.50	B
MOTA	4554	CA	GLY		20	69.120	42.106	16.175	1.00 33.61	E
ATOM	4555,	c	GLY		20	69.575	40.663	16.175	1.00 33.98	E
	•				20	70.580	40.343	15.541	1.00 34.56	B
MOTA	4556	0	GLY					16.866	1.00 34.08	18
MOTA	4557	N	THR		21	68.847	39.789			B
MOTA	4558	CA	THR		21	69.198	38.372	16.897	1.00 35.71	
MOTA	4559	CB	THR	E	21	69.193		18.335	1.00 37.69	E
ATOM	4560	OG1	THR	E	21	67.907	38.026	18.930	1.00 39.78	B
MOTA	4561	CG2	THR	B	21	70.268	38.480	19.174	1.00 38.05	E
ATOM	4562	C	THR	E	21	68.251	37.517	16.050	1.00 35.19	E
ATOM	4563	ō	THR		21	68.092	36.324	16.303	1.00 36.08	E
			GLU		22	67.619	38.129	15.052	1.00 34.15	B
ATOM	4564	N						14.176	1.00 34.08	E
ATOM	4565	CA	GLU		22	66.705	37.405			B
MOTA	4566	CB	GΓΩ		22	65.868	38.388	13.354	1.00 33.12	
ATOM	4567	CG	GLU	E	22	64.781	39.073	14.164	1.00 33.66	E
MOTA	4568	CD	GLU	E	22	64.173	40.266	13.451	1.00 35.85	E
MOTA	4569	OE	GLU	E	22	63.865	40.151	12.244	1.00 35.10	E
ATOM	4570		GLU		22	63.995	41.317	14.105	1.00 38.34	E
ATOM	4571	C.	GLU		22	67.523	36.503	13.265	1.00 33.80	E
						67.205	35.329	13.092	1.00 34.50	E
MOTA	4572	0	GLU		22				1.00 33.59	E
ATOM	4573	N	ARG		23	68.574	37.065	12.678		
MOTA	4574	CA	ARG		23	69.467	36.298	11.818	1.00 33.75	E
MOTA	4575	CB	ARG	E	23	69.703	36.996	10.470	1.00 36.33	E
MOTA	4576	ÇG	ARG	E	23	68.599	36.815	9.434	1.00 42.06	B
MOTA	4577	æ	ARG		23	67.342	37.577	9.813	1.00 47.83	E
ATOM	4578	NE	ARG		23	66.408	37.696	8.695	1.00 51.02	B
ATOM	4579	CZ	ARG		23	65.349	38.502	8.690	1.00 52.66	B
						65.087	39.263	9.747	1.00 50.82	E
MOTA	4580		L ARG		23				1.00 53.53	E
MOTA	4581	NH			23	64.555	38.555	7.626		E
ATOM	4582	C	ARG		23	70.788	36.177	12.560	1.00 30.98	
MOTA	4583	0	ARG	R	23	71.465	37.172	12.827	1.00 30.90	E

MOTA	4584	N	VAL I	В	24	71.149	34.955	12.909	1.00 28.33	B
ATOM	4585	CA	VAL I	E	24	72.394	34.735	13.621	1.00 25.06	B
ATOM	4586	CB	VAL :		24	72.148	34.500	15.129	1.00 22.98	B
ATOM	4587		VAL		24	73.456	34.106	15.817	1.00 21.05	E
ATOM	4588		VAL :		24	71.582	35.762	15.763	1.00 21.04	E
MOTA	4589	C	VAL		24	73.144	33.550	13.049	1.00 23.08	B
			VAL :		24	72.600	32.458	12.914	1.00 24.17	E
MOTA	4590	0				74.398		12.694	1.00 23.02	E
MOTA	4591	N	ARG		25		33.778		1.00 23.30	B
ATOM	4592	CA	ARG		25	75.223	32.718	12.156		
ATOM	4593	CB	ARG		25	75.511	32.930	10.659	1.00 24.06	E
ATOM	4594	CG	ARG	B	25	76.653	32.044	10.176	1.00 25.99	E
ATOM	4595	CD	ARG	E	25	76.470	31.478	8.774	1.00 28.29	E
ATOM	4596	NB	ARG	В	25	76.468	32.502	7.743	1.00 29.69	E
ATOM	4597	CZ	ARG	B	25	76.786	32.287	6.466	1.00 29.57	E
ATOM	4598	NH1	ARG	B	25	77.145	31.075	6.047	1.00 27.28	E
ATOM	4599		ARG		25	76.733	33.293	5.604	1.00 26.98	B
ATOM	4600	C	ARG		25	76.535	32.631	12.916	1.00 22.65	E
ATOM	4601	ŏ	ARG		25	77.261	33.620	13.041	1.00 22.47	E
ATOM	4602	N	LEU		26	76.828	31.444	13.433	1.00 21.04	B
			LEU		26	78.069	31.227	14.152	1.00 21.94	B
MOTA	4603	CA				77.834	30.338	15.383	1.00 21.37	B
MOTA	4604	СВ	TEO		26				1.00 22.89	E
MOTA	4605	CG	LEU		26	79.054	29.778	16.128		E
MOTA	4606		LEU		26	78.723	29.567	17.602	1.00 25.16	
MOTA	4607	CD2	TEG		26	79.483	28.466	15.493	1.00 23.51	B
MOTA	4608	C	ΓEΩ	E	26	79.032	30.552	13.193	1.00 21.17	E
ATOM	4609	0	LEU	E	26	78.637	29.674	12.432	1.00 21.77	E
ATOM	4610	N	VAL	E	27	80.285	30.983	13.201	1.00 19.92	E
ATOM	4611	CA	VAL	E	27	81.278	30.358	12.345	1.00 21.31	E
ATOM	4612	CB	VAL	B	27	81.530	31.166	11.039	1.00 20.44	E
ATOM	4613		VAL		27	82.524	30.420	10.156	1.00 21.63	B
ATOM	4614		VAL		27	80.221	31.366	10.275	1.00 20.48	E
ATOM	4615	c	VAL		27	82.581	30.231	13.112	1.00 21.74	B
ATOM	4616	ŏ	VAL		27	83.189	31.228	13.487	1.00 24.11	E
		N	SER		28	82.994	29.001	13.383	1.00 20.88	B
MOTA	4617				28	84.249	28.799	14.084	1.00 21.53	E
MOTA	4618	CA	SER			84.113	27.702	15.152	1.00 20.62	B
MOTA	4619	CB	SER		28			14.598	1.00 29.22	E
MOTA	4620	QG	SER		28	83.693	26.475		1.00 21.41	E
MOTA	4621	C	SER		28	85.274	28.433	13.006		E
MOTA	4622	0	SER		28	84.992	27.631	12.105	1.00 19.11	
ATOM	4623	N	ARG	E	29	86.450	29.051	13.090	1.00 18.23	E
MOTA	4624	CA	ARG	E	29	87.496	28.838	12.105	1.00 18.45	E
ATOM	4625	CB	ARG	E	29	87.701	30.124	11.287	1.00 16.91	E
ATOM	4626	CG	ARG	E	29	86.433	30.817	10.810	1.00 17.70	E
ATOM	4627	œ	ARG	B	29	86.791	32.117	10.109	1.00 18.98	E
ATOM	4628	NE	ARG	E	29	85.631	32.902	9.705	1.00 20.82	E
ATOM	4629	CZ	ARG	E	29	84.939	32.704	8.586	1.00 22.76	E
MOTA	4630		ARG	E	29	85.285	31.739	7.743	1.00 21.05	E
ATOM	4631		ARG		29	83.904	33.482	8.309	1.00 20.13	E
ATOM	4632	C	ARG		29	88.842	28.435	12.710	1.00 18.44	E
ATOM	4633	ō	ARG		29	89.401	29.171	13.520	1.00 19.35	E
	4634	N	SER		30	89.351	27.269	12.315	1.00 18.98	E
MOTA	4635	CA	SER		30	90.657	26.788	12.774	1.00 21.70	E
MOTA				_	30	90.619	25.284	13.028	1.00 22.10	E
MOTA	4636	СВ	SER			89.718	24.969	14.072	1.00 27.24	E
MOTA	4637	OG	SER		30		27.119	11.639	1.00 23.03	E
MOTA	4638	C	SER		30	91.637			1.00 23.56	E
MOTA	4639	0	SER		30	91.509	26.604	10.528		
MOTA	4640	N	ILE		31	92.611	27.978	11.927	1.00 23.05	E
MOTA	4641	CA	ILE		31	93.560	28.439	10.923	1.00 22.24	
MOTA	4642	CB	ILE		31	93.563	29.997	10.856	1.00 22.84	E
MOTA	4643	CG:	2 ILE	E	31	94.163	30.470	9.545	1.00 19.19	E
ATOM	4644	CG:	LILE	E	31	92.143	30.546	11.043	1.00 24.76	E
MOTA	4645	CD :	l ILE	E	31	91.144	30.032	10.047	1.00 29.25	E
MOTA	4646	C	ILE	E	31	95.013	28.014	11.134	1.00 24.53	E
ATOM	4647	0	ILE		31	95.566	28.187	12.225	1.00 22.94	E
ATOM	4648	N	TYR		32	95.625	27.468	10.081	1.00 24.41	E
ATOM	4649	CA			32	97.030	27.089	10.120	1.00 24.27	E
ATOM	4650				32	97.277		9.417	1.00 26.61	E
ATOM	4651					98.733		9.444	1.00 29.24	E
ATOM	4652		l TYR			99.423		10.649	1.00 30.69	B
ATOM	4653		1 TYF			100.770		10.683	1.00 32.83	E
			2 TYP			99.426		8.267	1.00 31.46	B
MOTA	4654		2 TYF			100.774		8.288	1.00 32.58	E
MOTA	4655					101.438		9.497		E
MOTA	4656					102.768		9.522	1.00 33.44	E
MOTA	4657	OH	TYF	ι B	32	102.768	44.400	2.344		-

MOTA	4658	C	TYR	E	32	97.700	28.225	9.353	1.00 24.83	E
MOTA	4659	0	TYR		32	97.444	28.415	8.164	1.00 25.49	E
MOTA	4660	N	ASN		33	98.543	28.985 30.146	9.461	1.00 24.28 1.00 24.25	e
MOTA MOTA	4661 4662	CA CB	asn asn		33 33	99.202 100.144	29.740	8.324	1.00 23.93	B
ATOM	4663	CG	ASN		33	101.379	29.014	8.834	1.00 25.26	B
ATOM	4664		ASN		33	102.003	29.439	9.808	1.00 26.40	B
MOTA	4665	ND2	asn	E	33	101.737	27.918	8.181	1.00 25.47	B
MOTA	4666	C	ASN		33	98.114	31.099	8.980	1.00 24.88	R
MOTA	4667	0	ASN		33	97.494	31.780 31.163	9.799 7.677	1.00 25.88 1.00 24.52	e
ATOM ATOM	4668 4669	n Ca	ARG ARG		34 34	97.864 96.815	32.055	7.194	1.00 26.32	E
ATOM	4670	CB	ARG		34	97.385	33.175	6.317	1.00 26.61	E
ATOM	4671	CG	ARG		34	97.999	34.346	7.072	1.00 26.37	E
MOTA	4672	ස	ARG	E	34	97.776	35.646	6.304	1.00 28.18	E
MOTA	4673	NE	ARG		34	97.886	35.429	4.865	1.00 31.86 1.00 33.42	e
MOTA	4674	CZ	ARG ARG		34 34	97.607 97.197	36.332 37.550	3.931 4.265	1.00 35.42	E
MOTA MOTA	4675 4676		ARG		34	97.722	36.003	2.653	1.00 35.29	B
ATOM	4677	c	ARG		34	95.728	31.333	6.417	1.00 26.98	E
MOTA	4678	0	ARG	B	34	94.896	31.968	5.763	1.00 28.88	E
MOTA	4679	N	GLU		35	95.719	30.010	6.481	1.00 26.13	e
ATOM	4680	CA	GLU		35	94.698	29.279 28.359	5.759 4.720	1.00 27.02 1.00 31.96	E
MOTA	4681 4682	CB CG	GLU GLU		35 35	95.350 96.284	27.301	5.278	1.00 38.52	B
ATOM ATOM	4683	CD	GLU		35	97.116	26.633	4.192	1.00 42.24	E
ATOM	4684		GLU		35	98.180	27.187	3.832	1.00 44.86	E
MOTA	4685	OE2			35	96.699	25.565	3.690	1.00 43.70	E
MOTA	4686	C	GLU		35	93.754	28.498	6.671	1.00 25.31 1.00 22.18	e
MOTA	4687	0	GLU		35 36	94.175 92.464	27.709 28.756	7.522 6.498	1.00 24.46	E
MOTA MOTA	4688 4689	N CA	GLU		36	91.438	28.085	7.272	1.00 24.13	E
ATOM	4690	СВ	GLU		36	90.085	28.731	7.001	1.00 24.37	E
ATOM	4691	CG	GLU	E	36	88.975	28.295	7.928	1.00 25.26	E
MOTA	4692	CD	GLU		36	87.669	28.991	7.604	1.00 26.01	E
ATOM	4693		GLU		36	87.672	29.847 28.689	6.694 8.253	1.00 27.25 1.00 27.12	E
ATOM	4694 4695	C C	GLU		36 36	86.646 91.413	26.630	6.826	1.00 23.40	B
ATOM ATOM	4696	o	GLU		36	91.252	26.347	5.645	1.00 23.72	E
ATOM	4697	N	ILE		37	91.576	25.707	7.767	1.00 23.97	E
ATOM	4698	CA	ILE		37	91.579	24.294	7.419	1.00 24.33	E
MOTA	4699	CB	ILE		37	92.818	23.578	8.019 7.532	1.00 24.98 1.00 24.26	e
MOTA	4700		ILE ILE		37 37	94.096 92.771	24.255 23.616	9.544	1.00 25.10	B
MOTA MOTA	4701 4702		IL		37	93.822	22.742	10.204	1.00 26.49	E
ATOM	4703	c	IL		37	90.301	23.555	7.836	1.00 23.49	E
MOTA	4704	0	IL	B	37	89.871	22.627	7.162	1.00 23.62	B
MOTA	4705	N	VAI		38	89.690	23.975	8.936	1.00 25.16	E
ATOM	4706	CA	VAI		38	88.465 88.715	23.342 22.489	9.415 10.667	1.00 25.85 1.00 26.44	E
MOTA MOTA	4707 4708	CB	VAI L VAI		38 38	87.516	21.610	10.932	1.00 27.10	E
ATOM	4709		VA		38	89.980	21.671	10.495	1.00 29.59	E
ATOM	4710	C		E	38	87.481	24.428	9.792	1.00 24.45	E
MOTA	4711	0		LE	38	87.885	25.471	10.288	1.00 24.36 1.00 24.90	B
MOTA	4712	И		3 B	39	86.193 85.175	24.168 25.161	9.594 9.904	1.00 24.90	E
ATOM ATOM	4713 4714	CA CB		3 B 3 B	39 39	84.975	26.055	8.678	1.00 25.55	E
MOTA	4715	CG		3 E		83.956	27.174	8.857	1.00 29.11	E
MOTA	4716	CD		g E		83.514	27.755	7.515	1.00 29.37	E
ATOM	4717	NE		G E		84.626	28.289	6.739	1.00 29.70	E
MOTA	4718	CZ		G E		84.505 83.314			1.00 31.37 1.00 33.54	E
ATOM	4719		1 AR 2 AR			85.572				E
MOTA MOTA	4720 4721			GE		83.813			1.00 23.51	E
ATOM	4722			G E		83.385	23.539	9.853	1.00 23.83	E
MOTA	4723	N		B E		83.147				E
MOTA	4724			E E		81.799				E
MOTA	4725			e e e e		81.682 80.296				Ē
MOTA MOTA	4726 4727		1 PH			79.944				E
MOTA	4728		2 PH			79.315			1.00 16.82	E
MOTA	4729	CE	1 PH	E F	40	78.628				E
MOTA	4730	CE	2 PH			78.001				E
MOTA	4731	. CZ	PH	E	3 40	77.663	23.248	14.003	1.00 16.61	E

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MOTA	4732	C	PHE	E	40	80.938	26.148	11.395	1.00 21.77	B
ATOM	4733	0	DHR	B	40	81.064	27.167	12.071	1.00 20.81	E
MOTA	4734	N	ASP	В	41	80.067	26.033	10.404	1.00 21.82	E
MOTA	4735	CA	ASP		41	79.181	27.110	9.995	1.00 21.76	E
								8.470	1.00 22.62	E
MOTA	4736	CB	ASP		41	79.190	27.182			
MOTA	4737	CG	ASP	E	41	78.492	28.400	7.929	1.00 23.09	E
ATOM	4738	OD1	ASP	E	41	77.507	28.864	8.546	1.00 22.57	E
ATOM	4739		ASP		41	78.929	28.881	6.861	1.00 25.40	E
									1.00 21.43	B
ATOM	4740	С	ASP		41	77.801	26.713	10.493		
ATOM	4741	0	ASP	E	41	77.277	25.672	10.085	1.00 22.83	E
MOTA	4742	N	SER	E	42	77.210	27.520	11.369	1.00 19.04	B
ATOM	4743	CA	SER		42	75.896	27.173	11.895	1.00 20.39	B
								12.907	1.00 19.13	E
ATOM	4744	CB	SER		42	75.399	28.220			
MOTA	4745	OG	SER	E	42	75.271	29.505	12.323	1.00 24.30	E
ATOM	4746	C	SER	E	42	74.891	27.000	10.762	1.00 20.23	E
ATOM	4747	0	SER	B	42	73.916	26.267	10.910	1.00 18.97	E
	4748	N	ASP		43	75.145	27.660	9.631	1.00 21.77	E
ATOM										B
MOTA	4749	CA	ASP		43	74.261	27.556	8.470	1.00 24.99	
ATOM	4750	CB	ASP	В	43	74.561	28.651	7.439	1.00 26.10	E
ATOM	4751	CG	ASP	K	43	73.819	29.947	7.727	1.00 28.71	E
ATOM	4752		ASP		43	73.078	30.013	8.737	1.00 28.83	E
										E
ATOM	4753		ASP		43	73.976	30.902	6.939	1.00 31.35	
ATOM	4754	С	ASP	E	43	74.378	26.193	7.809	1.00 25.68	E
ATOM	4755	0	ASP	E	43	73.424	25.727	7.190	1.00 28.27	B
		N	VAL		44	75.544	25.558	7.937	1.00 25.47	B
ATOM	4756								1.00 23.51	E
MOTA	4757	CA	VAL		44	75.764	24.229	7.362		
MOTA	4758	CB	VAL	B	44	77.251	24.007	6.964	1.00 24.39	E
ATOM	4759	CG1	VAL	E	44	77.456	22.579	6.491	1.00 19.52	E
	4760		VAL		44	77.655	24.984	5.867	1.00 23.79	В
ATOM									1.00 23.25	E
MOTA	4761	С	VAL		44	75.356	23.154	8.373		
ATOM	4762	0	VAL	E	44	74.774	22.136	8.005	1.00 22.01	E
ATOM	4763	N	GLY	E	45	75.683	23.370	9.644	1.00 22.52	E
ATOM	4764	CA	GLY		45	75.292	22.411	10.664	1.00 21.82	E
							21.311	11.001	1.00 22.07	E
MOTA	4765	C	GLY		45	76.275				
MOTA	4766	0	GLY	E	45	75.982	20.442	11.818	1.00 22.49	E
ATOM	4767	N	GLU	B	46	77.439	21.317	10.373	1.00 22.18	E
MOTA	4768	CA	GLU	ĸ	46	78.421	20.295	10.691	1.00 23.77	E
			GLU		46	78.147	19.017	9.891	1.00 26.29	E
MOTA	4769	СВ								E
MOTA	4770	CG	GLU	E	46	78.455	19.112	8.411	1.00 28.23	
ATOM	4771	æ	GLU	E	46	78.214	17.795	7.677	1.00 32.67	E
ATOM	4772	OE1	GLU	E	46	78.575	17.706	6.482	1.00 33.19	B
ATOM	4773		GLU		46	77.661	16.855	8.290	1.00 33.19	E
								10.383	1.00 23.15	E
ATOM	4774	C	GLU		46	79.807	20.839			
ATOM	4775	0	GLU	E	46	79.943	21.880	9.747	1.00 23.06	E
ATOM	4776	N	PHE	E	47	80.835	20.153	10.857	1.00 21.79	E
ATOM	4777	CA	PHE		47	82.192	20.595	10.599	1.00 22.22	E
			PHE		47	83.175	19.864	11.515	1.00 22.30	E
ATOM	4778	CB								
MOTA	4779	CG	PHE		47 .	83.058	20.249	12.968	1.00 22.20	E
ATOM	4780	CD1	. PHE	E	47	83.867	21.246	13.508	1.00 19.80	E
MOTA	4781	CD2	PHE	E	47	82.151	19.598	13.802	1.00 23.06	B
ATOM	4782		PHE		47	83.781	21.585	14.858	1.00 18.93	E
									1.00 22.63	E
MOTA	4783		PHE		47	82.055	19.931	15.157		
MOTA	4784	CZ	PHE		47	82.872	20.925	15.684	1.00 20.81	E
MOTA	4785	C	PHE	E	47	82.513	20.278	9.147	1.00 24.14	E
MOTA	4786	0	PHE	E	47	82.064	19.258	8.609	1.00 23.25	E
			ARG		48	83.272	21.164	8.511	1.00 22.66	E
MOTA	4787	N						7.131	1.00 23.86	B
MOTA	4788	CA	ARG		48	83.672	20.966			
ATOM	4789	CB	ARG	E	48	82.801	21.795	6.181	1.00 23.48	E
MOTA	4790	CG	ARG	Ε	48	81.339	21.375	6.091	1.00 25.01	B
ATOM	4791	CD	ARG		48	81.155	20.061	5.348	1.00 25.08	E
					48	79.747	19.811	5.044	1.00 27.17	E
ATOM	4792	NE	ARG						1.00 29.38	E
MOTA	4793	CZ	ARG		48	79.038	20.515	4.164		
ATOM	4794	NH	LARG	E	48	79.604	21.513	3.498	1.00 31.36	E
ATOM	4795	NH	ARG	B	48	77.763	20.226	3.946	1.00 30.50	E
		C	ARG		48	85.119	21.395	6.972	1.00 24.13	E
MOTA	4796							7.416	1.00 25.58	B
MOTA	4797	0	ARG		48	85.507	22,480			
MOTA	4798	N	AL		49	85.924	20.537	6.360	1.00 22.26	E
MOTA	4799	CA	ALF	E	49	87.316	20.875	6.122	1.00 23.11	E
ATOM	4800	CB	ALA	E	49	88.102	19.630	5.711	1.00 22.46	E
	4801		AL			87.290	21.875	4.980	1.00 22.04	E
MOTA								4.048	1.00 23.16	B
MOTA	4802	0	AL			86.507	21.722		1.00 23.56	
MOTA	4803	N	VAI			88.108	22.916	5.050		E
MOTA	4804	CA	VAI	E	50	88.135	23.875	3.953	1.00 23.79	E
MOTA	4805		VAI			88.059	25.360	4.478	1.00 24.14	E
227 014	1003									

MOTA	4806	CG1	VAL	B	50	88.341	25.408	5.959	1.00 24.71	B
MOTA	4807		VAL		50	89.010	26.268	3.704	1.00 22.47	B
MOTA MOTA	4808 4809	C 0	VAL VAL		50 50	89.374 89.485	23.578 24.041	3.098 1.963	1.00 23.50 1.00 24.92	B
ATOM	4810	N	THR		51	90.281	22.770	3.650	1.00 24.49	B
ATOM	4811	CA	THR		51	91.492	22.317	2.951	1.00 25.50	E
MOTA	4812	CB	THR		51	92.742	23.198	3.234	1.00 25.69	E
ATOM	4813		THR		51	93.171	23.007	4.586	1.00 27.89	R
MOTA MOTA	4814 4815	CG2 C	THR THR		51 51	92.443 91.817	24.670 20.895	2.985 3.420	1.00 23.29 1.00 26.59	e
ATOM	4816	0	THR		51	91.387	20.477	4.496	1.00 27.35	E
ATOM	4817	N	TEA		52	92.576	20.154	2.617	1.00 28.03	E
ATOM	4818	CA	LEU		52	92.949	18.783	2.956	1.00 28.49	E
ATOM	4819	CB	FEA		52		·18.259 17.892	1.969 0.556	1.00 30.33 1.00 34.17	e e
ATOM ATOM	4820 4821	CG CD1	PEA PEA		52 52	93.536 94.749	17.628	-0.334	1.00 34.41	E
ATOM	4822		LEU		52	92.644	16.668	0.620	1.00 34.30	E
MOTA	4823	C	LEU		52	93.494	18.645	4.374	1.00 28.20	E
MOTA	4824	0	PEA		52	93.304	17.624	5.027	1.00 29.17	e B
ATOM ATOM	4825 4826	n Ca	LEU		53 53	94.179 94.766	19.677 19.682	4.839 6.171	1.00 28.30 1.00 28.75	E
MOTA	4827	CB	LEU		53	95.490	21.015	6.387	1.00 30.37	B
MOTA	4828	CG	LEU		53	96.939	21.010	6.882	1.00 32.74	E
MOTA	4829		LEU		53	97.777	20.085	6.008	1.00 31.60	E
MOTA	4830		LEU		53	97.498	22.444	6.854	1.00 30.06 1.00 27.82	e
MOTA MOTA	4831 4832	C 0	LEU		53 53	93.727 94.027	19.464 18.858	7.278 8.312	1.00 27.82	B
ATOM	4833	N	GLY		54	92.508	19.957	7.059	1.00 27.39	B
MOTA	4834	CA	GLY		54	91.466	19.813	8.062	1.00 26.92	E
ATOM	4835	C	GLY		54	90.569	18.589	7.949	1.00 28.33	E
MOTA MOTA	4836	N O	GLY		54 55	89.725 90.755	18.348 17.801	8.813 6.898	1.00 28.02 1.00 29.28	e
ATOM	4837 4838	CA	LEU		55	89.930	16.620	6.675	1.00 31.43	E
ATOM	4839	CB	LEU		55	90.410	15.885	5.419	1.00 32.39	E
MOTA	4840	CG	LEU		55	89.426	14.934	4.731	1.00 35.68	E
MOTA	4841		LEU		55 55	88.086	15.627	4.504 3.406	1.00 34.41 1.00 35.99	e
MOTA MOTA	4842 4843	CD2	PEA		55 55	90.018 89.865	14.473 15.659	7.867	1.00 32.09	B
ATOM	4844	ŏ	LEU		55	88.778	15.294	8.312	1.00 32.58	E
MOTA	4845	N	PRO		56	91.023	15.235	8.402	1.00 31.67	E
MOTA	4846	CD	PRO		56	92.411	15.520	8.000 9.546	1.00 31.37 1.00 31.17	e
ATOM ATOM	4847 4848	CA CB	PRO PRO		56 56	90.986 92.459	14.316 14.163	9.919	1.00 30.50	B
ATOM	4849	CG	PRO		56	93.161	14.352	8.611	1.00 31.19	E
MOTA	4850	C	PRO	E	56	90.158	14.865	10.708	1.00 31.43	E
ATOM	4851	0	PRO		56	89.250	14.195	11.205 11.138	1.00 32.17 1.00 29.94	E
MOTA MOTA	4852 4853	N CA	ALA ALA		57 57	90.473 89.748	16.086 16.709	12.244	1.00 28.45	E
ATOM	4854	СВ	ALA		5 <i>7</i>	90.314	18.098	12.532	1.00 27.09	E
ATOM	4855	C	ALA	E	57	88.249	16.807	11.960	1.00 27.57	E
ATOM	4856	0	ALA		57	87.436	16.466	12.812	1.00 26.57	E
MOTA	4857 4858	N CA	ALA ALA		58 58	87.899 86.505	17.270 17.422	10.761 10.349	1.00 27.40 1.00 28.85	E
MOTA MOTA	4859	CB	ALA		58	86.439	18.007	8.939	1.00 27.80	E
ATOM	4860	C	ALA		58	85.726	16.110	10,406	1.00 30.37	E
MOTA	4861	0	ALA		58	84.624	16.058	10.954	1.00 29.58	E
MOTA	4862	N	GLU		59 59	86.292 85.632	15.052 13.750	9.837 9.845	1.00 32.24 1.00 35.22	E
MOTA MOTA	4863 4864	CA CB	GLU		59	86.441	12.724	9.049	1.00 36.81	E
MOTA	4865	CG	GLU		59	86.392	12.917	7.549	1.00 40.89	. B
MOTA	4866	CD	GLU		59	87.057	11.775	6.805	1.00 44.28	E
ATOM	4867		GLU		59 59	88.291 86.342	11.597 11.052	6.955 6.075	1.00 45.76 1.00 45.12	B
MOTA MOTA	4868 4869	OE2	GLU		59	85.441	13.231	11.260	1.00 34.08	B
ATOM	4870	ō	GLU		59	84.384	12.697	11.596	1.00 34.48	E
MOTA	4871	N	TYF		60	86.466	13.387	12.090	1.00 33.21	B
ATOM	4872	CA	TYF		60	86.390	12.919	13.463 14.177	1.00 32.36 1.00 33.78	B
MOTA MOTA	4873 4874	CB	TYF		60 60	87.724 87.657	13.101 12.617	15.594	1.00 35.68	E
ATOM	4875		TY		60	87.543	11.259	15.872	1.00 37.48	E
ATOM	4876	CEI	TY	B	60	87.394	10.802	17.173	1.00 41.14	E
ATOM	4877		TY		60	87.628	13.514	16.655	1.00 37.26 1.00 40.26	E
MOTA MOTA	4878 4879	CE2	TYI TYI		60 60	87.478 87.360		17.965 18.218	1.00 41.88	E
ALUM	-013			_			·- -		· · · - -	

ATOM	4880	OH	TYR	E	60	87.198	11.262	19.508	1.00 44.51	B
ATOM	4881	C	TYR		60	85.312	13.623	14.275	1.00 32.30	B
ATOM	4882	0	TYR	E	60	84.430	12.976	14.839	1.00 30.56	E
MOTA	4883	N	TRP		61	85.391	14.950	14.347	1.00 31.42	E
MOTA	4884	CA	TRP		61	84.412	15.715	15.112	1.00 31.35	E
ATOM	4885	СВ	TRP		61	84.744	17.219	15.071	1.00 32.78	E
ATOM	4886	CC	TRP		61	86.051	17.584	15.748 15.425	1.00 35.14 1.00 37.07	E
MOTA MOTA	4887 4888	CB2	TRP		61 61	86.909 87.994	18.687 18.655	16.331	1.00 37.07	E
ATOM	4889	CE3	TRP		61	86.864	19.706	14.458	1.00 39.50	E
ATOM	4890		TRP		61	86.635	16.947	16.809	1.00 35.82	E
ATOM	4891		TRP		61	87.800	17.582	17.163	1.00 35.66	B
ATOM	4892	CZ2	TRP		61	89.034	19.602	16.300	1.00 38.95	E
MOTA	4893	CZ3	TRP	E	61	87.902	20.656	14.427	1.00 41.16	B
ATOM	4894	CH2	TRP	B	61	88.971	20.591	15.346	1.00 40.81	B
MOTA	4895	C	TRP	E	61	82.968	15.472	14.653	1.00 29.29	E
MOTA	4896	0	TRP		61	82.045	15.563	15.458	1.00 29.20	E
ATOM	4897	N	asn		62	82.772	15.162	13.373	1.00 27.86	E
ATOM	4898	CA	ASN		62	81.428	14.902	12.853	1.00 29.09	e
ATOM	4899	CB	asn asn		62 62	81.379 81.241	15.051 16.492	11.331 10.893	1.00 29.42 1.00 31.22	E
ATOM ATOM	4900 4901	CG	asn		62	80.563	17.288	11.545	1.00 29.56	E
ATOM	4902	ND2	ASN		62	81.870	16.834	9.772	1.00 31.73	E
ATOM	4903	C	ASN		62	80.906	13.519	13.220	1.00 28.26	H
ATOM	4904	ō	ASN		62	79.716	13.242	13.086	1.00 27.48	E
ATOM	4905	N	SER		63	81.795	12.647	13.672	1.00 27.47	E
ATOM	4906	CA	SER	E	63	81.381	11.311	14.056	1.00 29.39	E
ATOM	4907	CB	SER		63	82.511	10.310	13.803	1.00 28.56	B
MOTA	4908	OG	SER		63	83.607	10.545	14.671	1.00 32.72	B
ATOM	4909	C	SER		63	80.987	11.310	15.534	1.00 30.11	B
MOTA	4910	0	SER		63	80.515	10.297	16.055 16.196	1.00 31.52 1.00 28.86	E
ATOM	4911 4912	N CA	GLN GLN		64 64	81.173 80.834	12.453 12.604	17.612	1.00 28.28	E
MOTA MOTA	4912	CB	GLN		64	81.929	13.379	18.350	1.00 29.50	E
ATOM	4914	CG	GLN		64	83.330	12.787	18.266	1.00 29.72	E
ATOM	4915	æ	GLN		64	83.418	11.412	18.888	1.00 32.69	E
ATOM	4916		GLN		64	83.055	10.405	18.267	1.00 35.22	E
MOTA	4917	NB2	GLN	E	64	83.887	11.358	20.128	1.00 31.92	E
ATOM	4918	С	GLN	E	64	79.522	13.366	17.783	1.00 28.42	E
MOTA	4919	0	GLN		64	79.525	14.599	17.800	1.00 27.68	E
MOTA	4920	N	LYS		65	78.410	12.648	17.926	1.00 27.17	E
MOTA	4921	CA	LYS		65	77.111	13.300	18.097	1.00 29.82	e
ATOM	4922	CB	LYS		65 65	75.994 75.479	12.258 11.692	18.253 16.936	1.00 31.43 1.00 37.61	E
MOTA	4923 4924	CD	LYS		65 65	74.801	12.766	16.072	1.00 41.12	E
MOTA MOTA	4925	CE	LYS		65	73.489	13.267	16.696	1.00 44.25	E
ATOM	4926	NZ	LYS		65	72.832	14.322	15.861	1.00 44.10	B
ATOM	4927	C	LYS		65	77.067	14.273	19.278	1.00 28.07	E
ATOM	4928	0	LYS	E	65	76.406	15.308	19.211	1.00 27.46	E
ATOM	4929	N	ASP	B	66	77.758	13.938	20.361	1.00 27.40	E
ATOM	4930	CA	asp	E	66	77.783	14.809	21.532	1.00 26.85	B
ATOM	4931	CB	ASP		66	78.566	14.142	22.670	1.00 26.10	E
MOTA	4932	CG	ASP		66	79.899	13.576	22.212	1.00 29.25 1.00 28.95	e
MOTA	4933		ASP ASP		66 66	79.915 80.929	12.836 13.858	21.205 22.864	1.00 28.93	13
ATOM ATOM	4934 4935	C	ASP		66	78.390	16.174	21.193	1.00 26.21	E
ATOM	4936	Ö	ASP		66	77.844	17.215	21.559	1.00 26.58	E
ATOM	4937	N	ILE		67	79.510	16.170	20.478	1.00 26.25	E
MOTA	4938	CA	ILE		67	80.164	17.414	20.100	1.00 25.76	E
ATOM	4939	СВ	ILE		67	81.551	17.153	19.477	1.00 27.31	E
ATOM	4940		ILE		67	82.261	18.467	19.210	1.00 25.90	E
MOTA	4941		ILE		67	82.396	16.304	20.429	1.00 28.85	E
MOTA	4942		ILE		67	82.494	16.871	21.844	1.00 32.35	E
ATOM	4943	C	ILE		67	79.307	18.189	19.108	1.00 25.95	E
ATOM	4944	0	ILE		67	79.125	19.392	19.255	1.00 26.97 1.00 26.05	e
ATOM	. 4945	N CA	LEC		68 68	78.775 77.927	17.504 18.172	18.100 17.113	1.00 26.05	E
MOTA MOTA	4946 4947	CB	LEU		68	77.382	17.169	16.094	1.00 26.91	B
MOTA	4948	CG	LEU		68	78.154	16.987	14.790	1.00 27.01	E
MOTA	4949		LE		68	77.389	16.002	13.913	1.00 26.26	E
ATOM	4950		LEC		68	78.311	18.342	14.076	1.00 24.04	E
ATOM	4951	С	LEU	JE	68	76.760	18.870	17.792	1.00 26.03	E
MOTA	4952	0	LEU		68	76.433	20.011	17.465	1.00 25.76	B
MOTA	4953	N	GL	JE	69	76.134	18.175	18.737	1.00 27.50	E

75.000 18.726 19.471 1.00 30.38 ATOM 4954 CA GLU E 69 ATOM 4955 CB GLU E 69 74.481 17.720 20.508 1.00 34.06 B ATOM 4956 CG GLU E 69 73.426 16.742 19.989 1.00 40.55 ATOM 72.211 17.444 4957 CD GLUE 69 19.392 1.00 44.43 ATOM 4958 OB1 GLU E 69 71.802 18.505 19.922 1.00 43.73 ATOM 4959 OB2 GLU E 71.656 16.926 69 18.397 1.00 48.15 ATOM 4960 C GLU E 69 75.335 20.034 20.178 1.00 29.17 R ATOM 4961 GLU E 69 74.587 21.009 20.071 1.00 29.71 ٥ ATOM 4962 N ARG E 70 76.453 20.059 20.899 1.00 26.65 ATOM 4963 CA ARG E 70 76.844 21.262 21,620 1.00 25.51 ATOM 4964 CB ARG E 70 78.001 20.965 22.572 1.00 27.14 В ATOM 4965 CG ARG B 70 77.711 19.855 23.563 1.00 31.22 В ATOM 4966 CD ARG B 70 78.637 19.934 24.769 1.00 35.11 NE ARGE 70 78.758 18.647 ATOM 4967 25.440 1.00 39.19 R ATOM ARG E 70 79.456 17.628 4968 CZ 24.956 1.00 41.08 R MOTA 4969 NH1 ARG E 70 80.096 17.752 23.802 1.00 45.32 ATOM 4970 NH2 ARG E 70 79.511 16.486 25.618 1.00 44.01 ATOM 4971 C ARG E 70 77.230 22.395 20.677 1.00 24.57 76.927 23.557 77.897 22.057 ATOM 4972 ARG E 70 20.941 1.00 21.44 0 B LYS E 71 ATOM 4973 N 19.576 1.00 24.56 В ATOM 4974 CA LYS E 71 78.309 23.071 18.612 1.00 24.08 ATOM 4975 CB LYS E 71 79.202 22.452 17.534 1.00 25.39 В ATOM 4976 CG LYS B 71 80.100 23.474 16.852 1.00 29.73 R ATOM 4977 CD LYS E 71 81.067 24.095 17.862 1.00 30.94 ATOM 4978 CE LYS B 71 81.905 25.205 17.256 1.00 31.82 ATOM 4979 NZ LYS E 71 82.774 25.849 18.290 1.00 33.45 В ATOM 77.087 23.732 17.960 1.00 22.42 77.045 24.951 17.780 1.00 18.65 LYS E 71 4980 C R LYS E 71 ATOM 4981 0 В ATOM 4982 N ARG E 72 76.092 22.919 17.620 1.00 22.31 ATOM 4983 CA ARG E 72 74.867 23.419 17.002 1.00 21.44 R CB ARG E 72 73.984 22.250 ATOM 4984 16.578 1.00 19.93 R ATOM 4985 CG ARG E 72 74.534 21.497 15.407 1.00 21.45 MOTA 4986 CD ARG E 72 73.779 20.223 15.141 1.00 23.34 NE ARGE 72 ATOM 4987 74.211 19.643 13.877 1.00 24.99 CZ ARG E 72 74.028 18.377 MOTA 13.522 1.00 27.42 4988 E NH1 ARG E 72 ATOM 4989 73.411 17.533 14.344 1.00 25.90 E MOTA 4990 NH2 ARG E 72 74.475 17.955 12.341 1.00 25.41 74.093 24.315 ATOM 4991 C ARG E 72 17.961 1.00 21.34 ARG E 72 73.336 25.182 MOTA 4992 0 17.535 1.00 23.67 B ALA E 73 ATOM 74.293 24.105 19.256 1.00 21.13 4993 N CA ALA E 73 MOTA 4994 73.610 24.887 20.281 1.00 22.11 E CB ALA E 73 73.476 24.052 21.568 1.00 21.20 MOTA 4995 ALA E 73 74.347 26.189 20.576 1.00 22.67 MOTA 4996 C E ALA E 73 4997 73.773 27.133 MOTA 0 21.125 1.00 25.58 E MOTA 4998 N ALA E 74 75.614 26.248 20.195 1.00 22.52 CA ALA B 74 76.420 27.432 20.448 MOTA 4999 1.00 22.20 CB ALA E 74 MOTA 5000 77.830 27.219 19.910 1.00 24.81 5001 ALA E 74 75.828 28.722 19.882 1.00 22.28 MOTA C Е MOTA 5002 0 ALA B 74 76.027 29.796 20.452 1.00 20.24 E VAL B 75 MOTA 5003 N 75.102 28.634 18.770 1.00 21.92 CA VAL E 75 74.519 29.841 18.185 1.00 21.69 ATOM 5004 E CB VAL E 75 73.700 29.517 16.890 1.00 22.61 MOTA 5005 Е MOTA 5006 CG1 VAL E 75 72.488 28.657 17.219 1.00 24.39 MOTA 5007 CG2 VAL E 75 73.270 30.798 16.218 1.00 24.00 Е VAL E 75 MOTA 5008 C 73.639 30.558 19,219 1.00 21.26 Е 5009 VAL E 75 MOTA O 73.464 31.777 19.164 1.00 20.64 MOTA 5010 N ASP B 76 73.106 29.802 20.171 1.00 20.84 MOTA 5011 CA ASP E 76 72.273 30.385 21.220 1.00 23.98 CB ASP B 76 MOTA 5012 71.022 29.532 21.471 1.00 25.33 Е ATOM 5013 CG ASP E 76 70.010 29.605 20.331 1.00 27.46 E MOTA 5014 OD1 ASP B 76 69.807 30.697 19.763 1.00 29.45 5015 OD2 ASP E MOTA 76 69.398 28.566 20.020 1.00 31.17 5016 C ASP E 73.044 30.525 22.538 MOTA 76 1.00 24.46 ASP E 76 72.910 MOTA 5017 0 31.524 23.247 1.00 25.64 R MOTA 5018 N ARG E 77 73.846 29.515 22.855 1.00 23.56 E MOTA 5019 CA ARG E 77 74.627 29.486 24.085 1.00 22.99 MOTA 5020 CB ARG E 75.176 28.077 24.279 1.00 26.55 77 ATOM 5021 CG ARG E 77 75.848 27.806 25.607 1.00 33.45 E ARG E 77 5022 MOTA CD 75.961 26.295 25.825 1.00 37.66 MOTA 5023 NE ARGE 77 74.639 25.666 25.883 1.00 40.99 CZ ARG E 77 ATOM 5024 74.423 24.352 25.862 1.00 43.13 ATOM 5025 NH1 ARG E 77 75.438 23.503 25.782 1.00 43.11 5026 NH2 ARG B 77 25.914 1.00 44.93 ATOM 73.183 23.885 5027 C ARG E 77 MOTA 75.763 30.509 24.078 1.00 23.23

ATOM 5028 O ARG E 77 76.162 31.022 25.129 1.00 23.14 B ATOM VAL E 78 5029 N 76.275 30.808 22.889 1.00 20.54 5030 CA VAL E 78 ATOM 77.354 31.767 22.741 1.00 19.56 ATOM 5031 CB VAL E 78 78.500 31.181 21.891 1.00 19.17 5032 CG1 VAL E 78 ATOM 79.612 32.208 21.724 1.00 17.69 ATOM 5033 CG2 VAL E 78 79.032 29.921 22.541 1.00 19.40 MOTA 5034 C VAL E 78 76.888 33.075 22.093 1.00 19.95 76.786 34.110 ATOM VALE 78 5035 0 22.756 1.00 21.57 ATOM 5036 CYS E 79 N 76.595 33.021 20.799 1.00 17.88 ATOM CA CYS E 79 5037 76.181 34.205 20.059 1.00 17.48 ATOM 5038 C CYS E 79 74.967 34.966 20,620 1.00 18.40 5039 O CYS E 79 5040 CB CYS E 79 MOTA 75.087 36.146 75.946 33.847 20.967 1.00 16.69 R MOTA 18.592 1.00 17.30 R ATOM 5041 SG CYS E 79 77.361 33.071 17.722 1.00 27.04 E ARG E 80 73.802 34.326 MOTA 5042 N 20.717 1.00 17.59 ATOM 5043 CA ARG E 80 72.641 35.050 21.240 1.00 20.01 E 5044 CB ARG E 80 ATOM 71.340 34.256 21.032 1.00 20.22 E 70.886 34.213 19.584 1.00 22.92 69.423 33.811 19.439 1.00 23.91 MOTA 5045 CG ARG E 80 MOTA 5046 CD ARG E 80 5047 NE ARG E 80 68.972 33.965 18.057 1.00 23.49 MOTA E ATOM CZ ARG E 80 69.206 33.089 17.082 1.00 25.16 E ATOM 5049 NH1 ARG B 80 69.884 31.975 17.326 1.00 24.15 ATOM 68.778 33.336 15.851 1.00 25.51 72.804 35.423 22.716 1.00 20.35 5050 NH2 ARG E 80 MOTA 5051 C ARG E 80 В 5052 O 72.317 36.464 23.153 1.00 17.98 ARG E 80 MOTA В ATOM 5053 N HIS E 81 73.495 34.581 23.479 1.00 21.22 73.717 34.867 24.895 CA HIS E 81 ATOM 5054 1.00 22.79 ATOM 5055 CB HIS E 81 74.467 33.717 25.572 1.00 24.38 ATOM CG HIS E 81 5056 74.955 34.046 26.950 1.00 26.42 E CD2 HIS E 81 ATOM 5057 76.188 34.381 27.404 1.00 26.61 E MOTA 5058 ND1 HIS E 81 74.122 34.080 28.048 1.00 26.60 ATOM 5059 CE1 HIS B 81 74.819 34.420 29.117 1.00 25.75 E ATOM 5060 NE2 HIS E 81 76.075 34.609 28.754 1.00 26.16 E 74.531 36.146 25.060 74.109 37.076 25.742 ATOM 5061 C HIS E 81 1.00 21.41 ATOM 5062 O HIS E 81 1.00 19.84 ASN E 82 MOTA 5063 N 75.700 36.188 24.426 1.00 22.13 ATOM 5064 CA ASN E 82 76.568 37.361 24.535 1.00 21.51 E ATOM 5065 CB ASN R 82 77.927 37.111 23.864 1.00 18.47 В CG ASN E 82 OD1 ASN E 82 ATOM 5066 78.702 35.982 24.515 1.00 18.09 ATOM 5067 78.453 35.632 25.669 1.00 19.05 5068 · ND2 ASN B 82 ATOM 79.656 35.409 23.777 1.00 15.06 75.936 38.612 23.949 1.00 20.33 76.212 39.716 24.412 1.00 22.84 ATOM 5069 C ASN E 82 1.00 20.33 5070 O ASN E 82 MOTA TYR E 83 MOTA 5071 N 75.089 38.454 22.940 1.00 19.71 MOTA 5072 CA TYR E 83 74.454 39.620 22.336 1.00 20.96 ATOM 5073 CB TYR E 83 73.619 39.211 21.114 1.00 21.58 Е MOTA 5074 CG TYR E 83 73.223 40.368 20.218 1.00 22.56 MOTA 5075 CD1 TYR E 83 72.047 41.090 20.439 1.00 23.70 5076 CE1 TYR E 83 ATOM 71.682 42.152 19.593 1.00 25.46 74.027 40.736 19.140 1.00 22.35 73.675 41.788 18.297 1.00 24.48 MOTA 5077 CD2 TYR E 83 5078 CE2 TYR E 83 ATOM 5079 CZ TYR E 83 ATOM 72.508 42.491 18.523 1.00 26.06 72.185 43.524 17.671 1.00 28.63 73.583 40.345 23.363 1.00 21.22 ATOM 5080 OH TYR E 83 R 5081 C ATOM TYR E 83 Е ATOM 5082 O TYR E 83 73.399 41.557 23.276 1.00 21.25 5083 N MOTA GLN B 84 73.046 39.606 24.333 1.00 22.94 MOTA 5084 CA GLN B 84 72.234 40.226 25.377 1.00 25.07 MOTA 5085 CB GLN B 84 71.631 39.180 26.324 1.00 25.76 ATOM 5086 CG GLN B 84 70.863 38.047 25.653 1.00 30.97 5087 CD GLN E 84 MOTA 69.889 38.525 24.594 1.00 33.95 ATOM 5088 OE1 GLN E 84 69.055 39.401 24.840 1.00 36.35 69.986 37.940 23.401 1.00 36.25 MOTA 5089 NE2 GLN E 84 5090 C ATOM GLN E 84 73.158 41.145 26.174 1.00 25.41 ATOM 5091 0 GLN B 84 72.804 42.290 26.473 1.00 27.11 5092 ท MOTA LEU E 85 74.344 40.637 26.510 1.00 24.17 75.330 41.413 27.256 1.00 26.47 76.601 40.590 27.515 1.00 26.91 ATOM 5093 CA LEU E 85 E 5094 CB LEU E 85 ATOM ATOM 5095 CG LEU E 85 76.485 39.202 28.161 1.00 29.65 5096 CD1 LEU E 85 ATOM 77.872 38.735 28.587 1.00 31.29 MOTA 5097 CD2 LEU E 85 75.564 39.247 29.365 1.00 32.27 75.698 42.661 26.459 1.00 26.89 75.762 43.757 27.004 1.00 28.24 ATOM 5098 С LEU B 85 ATOM 5099 O LEU B 85 5100 N 5101 CA MOTA GLU E 86 75.941 42.484 25.162 1.00 27.39 MOTA GLUE 86 76.293 43.603 24.295 1.00 28.02

ATOM	5102	СВ	GLU	E	86	76.492	43.126	22.852	1.00 26.60	B
MOTA	5103	CG	GLΨ	E	86	77.524	42.026	22.672	1.00 30.65	B
MOTA	5104	CD	GLU		86	78.942	42.457	23.024	1.00 31.17	E
MOTA	5105		GLU		86	79.860	41.612	22.919	1.00 31.68	B
ATOM	5106		GLU		86	79.139	43.631	23.402	1.00 31.77	E
ATOM	5107	C	GLU		86	75.165	44.630	24.327	1.00 27.95 1.00 24.30	e
MOTA	5108	0	GLU		86 87	75.407 73.935	45.834 44.130	24.257 24.442	1.00 24.30	E
ATOM ATOM	5109 5110	N CA	LEU		87	72.736	44.962	24.468	1.00 28.30	B
ATOM	5111	CB	PEA		87	71.496	44.062	24.423	1.00 32.64	E
ATOM	5112	CG	LEU		87	70.506	44.100	23.248	1.00 35.59	B
ATOM	5113		LEU		87	71.101	44.734	21.997	1.00 35.24	E
MOTA	5114		LEU		87	70.071	42.675	22.965	1.00 34.35	E
MOTA	5115	C	LEU	B	87	72.669	45.893	25.686	1.00 33.33	E
ATOM	5116	0	LEU	E	87	71.967	46.902	25.663	1.00 32.52	E
MOTA	5117	N	ARG		88	73.401	45.560	26.745	1.00 35.06	E
MOTA	5118	CA	ARG		88	73.399	46.389	27.948	1.00 37.29	E
ATOM	5119	CB	ARG		88	73.348	45.524	29.215	1.00 39.69	E
ATOM	5120	CG	ARG		88	72.471	44.275	29.158 30.529	1.00 43.37 1.00 45.38	B
ATOM	5121	CD NE	ARG ARG		88 88	72.441 71.846	43.592 42.257	30.499	1.00 48.76	E
MOTA MOTA	5122 5123	CZ	ARG		88	70.625	41.985	30.047	1.00 50.95	E
ATOM	5124		ARG		88	69.854	42.958	29.579	1.00 52.23	E
ATOM	5125		ARG		88	70.171	40.738	30.064	1.00 51.26	E
ATOM	5126	C	ARG	E	88	74.670	47.225	28.010	1.00 37.36	E
ATOM	5127	0	ARG	E	88	74.842	48.044	28.913	1.00 37.55	E
ATOM	5128	N	THR	E	89	75.564	47.019	27.049	1.00 36.40	B
MOTA	5129	CA	THR		89	76.834	47.731	27.055	1.00 34.93	B
ATOM	5130	CB	THR		89	77.951	46.807	27.590	1.00 36.26	E
ATOM	5131		THR		89	77.973	45.590	26.825	1.00 34.21	E
ATOM	5132	CG2			89	77.708	46.478	29.056 25.718	1.00 33.95 1.00 33.37	E
MOTA	5133	C	THR		89 89	77.294 76.958	49.431	25.356	1.00 33.30	E
ATOM ATOM	5134 5135	И	THR		90	78.080	47.510	25.000	1.00 32.11	E
ATOM	5136	ÇA	THR		90	78.639	47.895	23.712	1.00 30.45	B
ATOM	5137	CB	THR		90	79.313	46.681	23.041	1.00 31.20	E
ATOM	5138		THR		90	80.238	46.086	23.958	1.00 32.67	E
ATOM	5139	CG2	THR	E	90	B0.076	47.109	21.811	1.00 32.64	E
ATOM	5140	C	THR	E	90	77.639	48.504	22.738	1.00 28.40	E
ATOM	5141	0	THR		90	77.903	49.538	22.133	1.00 27.20	B
ATOM	5142	N	LEU		91	76.489	47.864	22.582	1.00 29.83	E
ATOM	5143	CA	LEU		91	75.482	48.361	21.655	1.00 29.52 1.00 27.50	E
ATOM	5144	CB	LEU		91	74.474 75.091	47.252 46.101	21.354 20.550	1.00 27.30	E
ATOM	5145 5146	CG	LEU		91 91	74.102	44.959	20.457	1.00 24.51	B
MOTA MOTA	5147		LEU		91	75.487	46.593	19.157	1.00 23.04	E
ATOM	5148	C	LEU		91	74.770	49.629	22.129	1.00 30.74	E
MOTA	5149	ō	LEU		91	73.994	50.228	21.382	1.00 31.46	E
MOTA	5150	N	GLN	E	92	75.035	50.043	23.366	1.00 29.33	E
MOTA	5151	CA	GLN	E	92	74.427	51.259	23.884	1.00 30.04	E
ATOM	5152	CB	GLN		92	73.869	51.044	25.294	1.00 31.55	E
MOTA	5153	CG	GLN		92	72.500	50.381	25.327	1.00 36.90	E
MOTA	5154	CD	GLN		92	71.865	50.426	26.706	1.00 41.59	E
MOTA	5155		GLN		92	70.760	49.920	26.911 27.662	1.00 43.76 1.00 43.75	e
MOTA	5156	NE2	GLN GLN		92 92	72.563 75.430	51.037 52.409	23.898	1.00 28.45	E
MOTA MOTA	5157 5158	Ö	GLN		92	75.059	53.558	24.125	1.00 28.57	B
MOTA	5159	N	ARG		93	76.699	52.098	23.650	1.00 26.37	E
ATOM	5160	CA	ARG		93	77.737	53.127	23.633	1.00 26.74	E
ATOM	5161	CB	ARG		93	79.112	52.513	23.340	1.00 24.84	E
ATOM	5162	CG	ARG		93	80.260	53.525	23.217	1.00 20.15	B
MOTA	5163	CD	ARG	E	93	81.569	52.801	22.894	1.00 20.06	E
MOTA	5164	NE	ARG		93	82.718	53.685	22.729	1.00 15.27	E
MOTA	5165	CZ	ARG		93	83.316	54.330	23.729	1.00 16.93	B
MOTA	5166		ARG		93	82.875	54.197	24.973	1.00 17.82	B
MOTA	5167		ARG		93	84.367	55.101 54.173	23.492 22.576	1.00 16.28 1.00 28.26	e
ATOM	5168 5169	C	ARG		93 93	77.428 77.202	54.173	22.576	1.00 28.26	E
MOTA MOTA	5169 5170	Ŋ	ARG		93 94	77.411	55.431	22.995	1.00 28.24	B
ATOM	5171	CA	ARG		94	77.159	56.529	22.084	1.00 29.74	E
ATOM	5172	CB	ARG		94	75.661	56.855	22.053	1.00 32.88	E
MOTA	5173	CG	ARC		94	74.912	55.941	21.086	1.00 36.76	E
MOTA	5174	CD	ARC		94	73.402	56.055	21.163	1.00 40.38	E
MOTA	5175	NE	ARC	B	94	72.758	55.304	20.080	1.00 44.16	E

MOTA 5176 CZ ARG B 94 72.871 53.991 19.894 1.00 43.57 ATOM 5177 NH1 ARG E 94 73.602 53.259 20.720 1.00 45.04 72.262 53.408 1.00 45.75 ATOM 5178 NH2 ARG R 94 18.869 R ATOM 5179 ARG E 94 77.992 57.734 22.497 1.00 29.26 77.773 ATOM 5180 0 ARG E 94 58.331 23.546 1.00 30.32 VAL E 95 78.974 58.063 ATOM 5181 N 21,667 1.00 26.76 59.188 ATOM 5182 CA VAL E 95 79.859 21.936 1.00 25.75 MOTA CB VAL B 95 81.340 58.763 21.855 1.00 22.33 5183 MOTA CG1 VAL B 95 82.244 59.914 22.287 1.00 19.80 5184 CG2 VAL E 95 ATOM 5185 81.565 57.534 22.717 1.00 19.11 ATOM 5186 С VAL E 95 79.600 60.266 20.902 1.00 26.51 Е VAL B 95 79.787 60.042 19.703 1.00 27.04 ATOM 5187 0 GLU E 96 79.160 61.430 21.366 1.00 27.28 ATOM 5188 N CA GLU B 96 78.870 62.536 1.00 28.16 ATOM 5189 20.466 5190 CB GLU E 96 78.260 63.716 21.227 1.00 30.40 ATOM CG GLU E 96 ATOM 5191 76.965 63.396 21.952 1.00 34.36 5192 CD GLU E 96 76.348 64.625 22.609 1.00 36.84 ATOM E ATOM 5193 OE1 GLU E 96 75.295 64.478 23.272 1.00 38.81 ATOM OE2 GLU E 96 76.914 65.734 22.460 1.00 35.73 5194 В ATOM 5195 C GLU E 96 80.148 62.987 19.793 1.00 25.65 GLU E 96 81.176 63.171 1.00 24.93 ATOM 0 20.440 В 5196 ATOM 5197 N PRO E 97 80.101 63.168 18.473 1.00 25.41 Е ATOM 5198 CD PRO E 97 78.977 62.979 17.539 1.00 24.36 ATOM CA PRO E 97 81.304 63.603 17.770 1.00 24.81 5199 CB PRO E 97 80.927 63.416 16.306 1.00 24.85 ATOM 5200 E ATOM 5201 CG PRO E 97 79.456 63.717 16.309 1.00 25.36 R ATOM 5202 C PRO E 97 81.643 65.048 18.089 1.00 24.48 E PRO E 97 80.761 65.844 18.419 1.00 23.85 ATOM 5203 0 THR E 98 82.927 65.377 18.025 1.00 22.82 ATOM E 5204 N ATOM 5205 CA THR E 98 83.340 66.748 18.244 1.00 24.12 R THR E 98 84.679 66.852 19.019 1.00 26.31 ATOM 5206 CB MOTA OG1 THR E 98 85.744 66.355 18.205 1.00 34.47 5207 CG2 THR E 98 84.623 66.049 20.302 1.00 23.83 ATOM 5208 ATOM 5209 C THR E 98 83.519 67.254 16.817 1.00 22.12 E THRE 98 84.162 66.601 15.993 1.00 21.35 MOTA 5210 0 ATOM VAL E 99 82.923 68.400 16.516 1.00 21.99 5211 N CA VAL E 99 83.001 68.957 15.177 1.00 20.67 E ATOM 5212 1.00 19.57 ATOM 5213 CB VAL E 99 81.585 69.217 14.619 E CG1 VAL E 99 81.667 69.645 13.154 1.00 14.62 ATOM 5214 CG2 VAL E 99 80.732 67.944 14.766 1.00 15.20 MOTA 5215 VAL E 99 83.814 70.240 15.158 1.00 22.05 ATOM 5216 C MOTA 5217 0 VAL E 99 83.524 71.194 15.884 1.00 22.27 E ATOM 5218 N THR E 100 84.827 70.250 14.304 1.00 21.34 E ATOM CA THR E 100 85.728 71.376 14.176 1.00 23.10 5219 1.00 24.55 CB THR E 100 87.104 71.024 14.786 ATOM 5220 ATOM 5221 OG1 THR E 100 86.941 70.728 16.180 1.00 30.47 88.079 14.634 1.00 27.79 ATOM 5222 CG2 THR E 100 72.183 THR E 100 85.934 71.777 12.722 1.00 23.36 E ATOM 5223 С 11.842 1.00 21.77 86.024 70.926 MOTA 5224 0 THR E 100 ATOM 5225 ILE E 101 86.009 73.082 12.473 1.00 24.40 E N ATOM 5226 CA ILE E 101 86.236 73.584 11.124 1.00 25.31 85.092 74.518 10.645 1.00 24.21 CB ILE E 101 ATOM 5227 85.398 9.245 1.00 22.51 75.044 E MOTA 5228 CG2 ILE E 101 MOTA 5229 CG1 ILE E 101 83.760 73.768 10.636 1.00 24.86 82.584 1.00 25.22 MOTA 5230 CD1 ILE E 101 74.635 10.197 ILE E 101 87.538 74.372 11.116 1.00 26.66 ATOM 5231 C 87.859 75.065 12.074 1.00 26.18 ATOM 5232 O ILE E 101 ATOM 5233 **SER B 102** 88.287 74.262 10.029 1.00 31.17 ĸ N MOTA 5234 CA **SER B 102** 89.547 74.977 9.902 1.00 35.36 E SER B 102 90.619 74.306 10.755 1.00 34.20 ATOM 5235 CB 90.777 MOTA 5236 OG SER E 102 72.953 10.374 1.00 40.09 MOTA 5237 C **SER E 102** 89.976 74.979 8.448 1.00 36.82 89.913 7.777 1.00 36.68 ATOM 5238 0 SER E 102 73.953 MOTA PRO E 103 90.404 76.139 7.932 1.00 39.96 5239 N 90.458 77.473 8.553 1.00 40.07 ATOM 5240 Œ PRO E 103 6.532 1.00 42.01 E MOTA 5241 CA PRO E 103 90.831 76.190 PRO B 103 90.856 77.682 6.237 1.00 41.76 E ATOM 5242 CB MOTA 5243 CG PRO E 103 91.282 78.258 7.556 1.00 42.86 MOTA C 92,196 6.390 1.00 44.62 PRO E 103 75.534 5244 92.943 1.00 44.53 ATOM 5245 0 PRO E 103 75.430 7.365 ATOM SER E 104 92.514 75.086 5.181 1.00 47.92 5246 N 93.789 ATOM 5247 CA SER E 104 74.426 4.920 1.00 50.83 ATOM 93.712 1.00 52.33 SER E 104 73.637 3.612 5248 CB 94.904 72.901 3.396 1.00 55.60 ATOM SER E 104 5249 OG

ATOM	5250	C	SER E 104	94.941	75.422	4.845	1.00 52.18	В
MOTA	5251	0	SER E 104	96.080	75.093	5.186	1.00 53.53	E
ATOM	5252	N	ASN B 113	90.669	78.112	-1.692	1.00 48.40	B
ATOM	5253	CA	ASN E 113	90.651	77.795	-0.269	1.00 47.57	E
ATOM	5254	СВ	ASN E 113	89.863	78.854	0.496	1.00 51.34	E
ATOM	5255	CG	ASN E 113	90.504	80.219	0.417	1.00 52.99	E
ATOM	5256		L ASN E 113	90.693	80.765	-0.670	1.00 55.11	E
ATOM	5257		2 ASN E 113	90.845	80.781	1.572	1.00 55.09	B
ATOM	5258	C	ASN E 113	90.045	76.424	-0.001	1.00 44.87	B
ATOM	5259	0	ASN E 113	89.374	75.852	-0.860	1.00 44.99	E
ATOM	5260	N	LEU E 114	90.282	75.904	1.197	1.00 41.65	B
ATOM	5261	CA	LEU E 114	89.765	74.592	1.568	1.00 38.53	E
ATOM	5262	СВ	LEU B 114	90.823	73.521	1.287	1.00 38.84	E
ATOM	5263	CG	LEU E 114	90.383	72.060	1.441	1.00 40.32	· E
ATOM	5264		L LEU E 114	89.314	71.726	0.400	1.00 39.94	E
ATOM	5265		2 LEU E 114	91.586	71.145	1.266	1.00 40.52	B
ATOM	5266	C	LEU E 114	89.349	74.523	3.036	1.00 34.78	E
ATOM	5267	0	LEU E 114	90.173	74.684	3.929	1.00 33.51	E
ATOM	5268	N	LEU E 115	88.063	74.293	3.278	1.00 32.05	E
ATOM	5269	CA	LEU E 115	87.550	74.181	4.641	1.00 29.68	E
ATOM	5270	СВ	LEU E 115	86.158	74.809	4.754	1.00 29.84	E
ATOM	5271	CG	LEU B 115	86.046	76.257	5.241	1.00 31.52	E
ATOM	5272		LEU B 115	87.101	77.140	4.574	1.00 32.51	B
ATOM ATOM	5273		LEU E 115	84.636	76.762	4.948	1.00 30.75	E
ATOM	5274	C	LEU E 115	87.472	72.712	5.034	1.00 27.57	E
ATOM	5275	0	LEU E 115	86.871	71.900	4.331	1.00 25.33	E
ATOM	5276	N	VAL E 116	88.089	72.381	6.161	1.00 26.32	E
ATOM	5277 5278	CA CB	VAL E 116 VAL E 116	88.099	71.014	6.651	1.00 24.42	B
ATOM	5278 5279			89.513	70.572	7.075	1.00 24.51	E
ATOM	5280		VAL E 116	89.467	69.160	7.641	1.00 22.66	E
ATOM	5281	C	VAL E 116	90.458	70.643	5.879	1.00 26.70	E
ATOM	5282	Ö	VAL E 116	87.195	70.842	7.846	1.00 22.77	E
ATOM	5283	N	CYS E 117	87.376 86.208	71.496	8.868	1.00 23.04	E
ATOM	5284	CA	CYS E 117	85.326	69.968	7.717	1.00 22.34	E
ATOM	5285	C	CYS E 117	85.769	69.711	8.840	1.00 21.65	B
ATOM	5286	ō	CYS B 117	85.607	68.391 67.319	9.466 8.877	1.00 19.44	E
ATOM	5287	СВ	CYS E 117	83.863	69.626	8.401	1.00 18.95	B
ATOM	5288	SG	CYS E 117	82.771	69.420	9.844	1.00 22.57 1.00 25.79	E
ATOM	5289	N	SER E 118	86.355	68.488	10.654	1.00 25.79	e B
ATOM	5290	CA	SER E 118	86.837	67.330	11.387	1.00 17.98	E
ATOM	5291	CB	SER E 118	88.115	67.671	12.146	1.00 18.33	E
MOTA	5292	OG	SER E 118	89.121	68.117	11.260	1.00 24.58	E
ATOM	5293	C	SER E 118	85.798	66.860	12.377	1.00 17.01	E
MOTA	5294	0	SER E 118	85.507	67.543	13.354	1.00 16.69	E
MOTA	5295	N	VAL E 119	85.240	65.688	12.112	1.00 16.58	E
MOTA	5296	CA	VAL E 119	84.242	65.095	12.985	1.00 16.03	B
ATOM	5297	CB	VAL E 119	83.040	64.582	12.160	1.00 15.47	E
ATOM	5298	CG1	VAL E 119	81.918	64.147	13.077	1.00 13.75	E
ATOM	5299	CG2	VAL E 119	82.559	65.686	11.216	1.00 10.95	E
MOTA	5300	C	VAL E 119	85.018	63.960	13.638	1.00 17.51	E
ATOM	5301	0	VAL E 119	85.238	62.906	13.042	1.00 19.30	E
ATOM	5302	N	THR E 120	85.442	64.203	14.871	1.00 18.44	E
MOTA	5303	CA	THR E 120	86.265	63.266	15.616	1.00 18.41	E
MOTA	5304	CB	THR E 120	87.562	63.962	16.042	1.00 18.11	B
MOTA	5305		THR B 120	87.242	65.078	16.887	1.00 17.18	B
ATOM	5306		THR B 120	88.304	64.481	14.835	1.00 16.77	В
ATOM	5307	C	THR E 120	85.655	62.656	16.875	1.00 20.11	E
ATOM	5308	0	THR E 120	84.665	63.148	17.417	1.00 21.96	. В
ATOM	5309	N	ASP E 121	86.272	61.566	17.319	1.00 19.96	E
ATOM	5310	CA	ASP E 121	85.882	60.B64	18.529	1.00 21.06	E
ATOM	5311	CB	ASP E 121	86.313	61.686	19.745	1.00 25.93	E
ATOM	5312	CG	ASP E 121	87.814	61.765	19.882	1.00 30.02	E
ATOM	5313		ASP B 121	88.291	62.524	20.756	1.00 34.97	B
ATOM ATOM	5314		ASP E 121	88.513	61.063	19.114	1.00 31.15	E
ATOM	5315 5316	C	ASP E 121	84.431	60.463	18.709	1.00 20.39	E
ATOM ATOM	5316 5317	N O	ASP E 121	83.857	60.698	19.766	1.00 22.05	B
ATOM	5317	CA	PHE E 122 PHE E 122	83.827	59.841	17.708	1.00 19.69	E
ATOM	5319	СВ	PHE E 122	82.443 81.538	59.429	17.873	1.00 18.28	E
ATOM	5320	CG	PHE E 122	81.905	60.108	16.843	1.00 16.99	E
ATOM	5321		PHE E 122	82.770	59.821 60.661	15.417 14.725	1.00 16.67	B
ATOM	5322		PHE B 122	81.370	58.717	14.756	1.00 16.72 1.00 17.17	e
ATOM	5323		PHE E 122	83.096	60.410	13.384	1.00 17.17	B
				-3.000	40.470	~~ . JOZ	I.00 I/.00	_

2004	C204	ana	DITE -		07 606	CO 456	22 420		_
MOTA	5324		PHE E		81.686	58.456	13.419	1.00 16.82	B
ATOM	5325	CZ	PHE E		82.549	59.305	12.733	1.00 15.81	B
MOTA	5326	С	DHE E	122	82.287	57.925	17.774	1.00 18.35	E
ATOM	5327	0	PHE E	122	83.168	57.231	17.272	1.00 15.90	E
ATOM	5328	N	TYR E	123	81.157	57.436	18.276	1.00 19.49	E
MOTA	5329	CA	TYR E	123	80.818	56.021	18.243	1.00 20.92	B
ATOM	5330	CB	TYR E		81.523	55.261	19.374	1.00 21.02	E
MOTA	5331	CG	TYR E		81.387	53.762	19.247	1.00 20.05	E
MOTA	5332		TYR E		80.242	53.103	19.688	1.00 21.66	B
MOTA	5333		TYR F		80.095	51.726	19.516	1.00 21.85	E
ATOM	5334	CD2	TYR E	123	82.383	53.009	18.633	1.00 20.08	E
ATOM	5335	CE2	TYR E	123	82.250	51.643	18.455	1.00 19.20	E
ATOM	5336	\mathbf{cz}	TYR F	123	81.105	51.002	18.896	1.00 22.24	E
ATOM	5337	OH	TYR E		80.970	49.640	18.712	1.00 25.26	E
MOTA	5338	C	TYR E		79.311	55.957	18.440	1.00 21.42	B
MOTA	5339	0	TYR E		78.778	56.647	19.305	1.00 23.90	E
ATOM	5340	N	PRO E		78.609	55.100	17.676	1.00 20.39	E
ATOM	5341	CD	PRO E		77.155	54.937	17.844	1.00 21.24	E
MOTA	5342	CA	PRO F	124	79.113	54.177	16.655	1.00 21.61	B
MOTA	5343	CB	PRO E	124	77.956	53.188	16.500	1.00 19.35	B
ATOM	5344	CG	PRO E	124	76.776	54.056	16.670	1.00 19.34	E
MOTA	5345	C	PRO E		79.549	54.802	15.325	1.00 20.84	E
ATOM	5346	ō	PRO E		79.602	56.024	15.184	1.00 22.13	E
							14.361		E
MOTA	5347	N	ALA I		79.862	53.940		1.00 22.61	
MOTA	5348	CA	ALA I		80,329	54.341	13.027	1.00 25.48	B
ATOM	5349	CB	ALA E		80.860	53.121	12.288	1.00 26.06	E
ATOM	5350	C	ALA I	125	. 79.31 1	55.058	12.137	1.00 27.38	E
MOTA	5351	0	ALA I	125	79.681	55.906	11.332	1.00 29.08	E
ATOM	5352	N	GLN E	126	78.039	54.706	12.268	1.00 29.18	E
ATOM	5353	CA	GLN I		76.990	55.312	11.455	1.00 29.94	E
ATOM	5354	СВ	GLN I		75.625	54.737	11.848	1.00 33.48	E
			-						
ATOM	5355	CG	GLN I		75.536	53.200	11.840	1.00 39.27	E
ATOM	5356	CD	GLN I		76.067	52.537	13.117	1.00 41.92	E
MOTA	5357	OE1	GLN I	126	77.271	52.523	13.379	1.00 44.02	B
MOTA	5358	NE2	GLN I	126	75.159	51.981	13.913	1.00 43.83	E
ATOM	5359	C	GLN I	3 126	76.977	56.829	11.621	1.00 28.88	E
ATOM	5360	0	GLN I	3 126	76.739	57.331	12.719	1.00 28.83	E
ATOM	5361	N	ILE I		77.221	57.558	10.532	1.00 27.90	E
ATOM	5362	CA	ILE I		77.245	59.018	10.591	1.00 25.67	E
								1.00 25.23	E
ATOM	5363	CB	ILE 1		78.611	59.514	11.150		
MOTA	5364		ILE 1		79.693	59.398	10.084	1.00 21.16	E
MOTA	5365	CG1	IFE 1	3 127	78.504	60.965	11.610	1.00 22.40	E
ATOM	5366	CD1	ILE 1	3 127	79.610	61.376	12.546	1.00 25.35	E
MOTA	5367	С	ILE I	3 127	76.985	59.673	9.230	1.00 26.38	E
ATOM	5368	0	ILE I	3 127	77.196	59.065	8.182	1.00 26.20	E
ATOM	5369	N	LYS		76.521	60.916	9.252	1.00 25.64	E
			LYS		76.248	61.635	8.016	1.00 29.02	E
MOTA	5370	CA							
ATOM	5371	СВ	LYS	-	74.754	61.566	7.671	1.00 29.97	B
MOTA	5372	CG		3 128	74.408	62.178	6.317	1.00 35.17	E
MOTA	5373	CD		3 128	75.175	61.487	5.183	1.00 39.63	E
ATOM	5374	CE	LYS	3 128	74,936	62.163	3.836	1.00 41.20	B
ATOM	5375	NZ	LYS !	B 128	75.685	61.492	2.731	1.00 44.74	E
MOTA	5376	C	LYS :	E 128	76.683	63.090	8.154	1.00 28.40	E
ATOM	5377	0		3 128	76.203	63.812	9.028	1.00 27.15	E
ATOM	5378	N		B 129	77.600	63.506	7.287	1.00 28.99	Е
				B 129	78.119	64.866	7.304	1.00 29.32	E
MOTA	5379	CA							
MOTA	5380	CB		B 129	79.651	64.860	7.502	1.00 30.69	E
MOTA	5381		VAL :		80.171	66.282	7.654	1.00 27.54	E
MOTA	5382	CG2	VAL	B 129	80.014	64.012	8.721	1.00 30.82	E
MOTA	5383	C	VAL :	E 129	77.788	65.574	5.992	1.00 30.45	e
MOTA	5384	0	VAL :	B 129	78.042	65.039	4.915	1.00 30.36	E
MOTA	5385	N		B 130	77.221	66.775	6.090	1.00 31.17	E
MOTA	5386	CA		B 130	76.851	67.562	4.914	1.00 32.17	E
							4.764	1.00 34.73	B
ATOM	5387	СВ		E 130	75.330	67.626			
MOTA	5388	CG		E 130	74.632	66.335	4.400	1.00 40.85	E
MOTA	5389	СD		E 130	73.121	66.527	4.511	1.00 46.16	E
MOTA	5390	NE		E 130	72.365	65.456	3.864	1.00 51.33	E
MOTA	5391	CZ	ARG	E 130	71.046	65.308	3.959	1.00 53.45	B
MOTA	5392	NH1	ARG	E 130	70.327	66.162	4.680	1.00 54.21	K
ATOM	5393		ARG		70.444	64.307	3.329	1.00 53.97	E
ATOM	5394	C		E 130	77.359	68.994	5.017	1.00 30.88	B
MOTA	5395	o		B 130	77.321	69.590	6.093	1.00 30.84	B
								1.00 29.14	E
MOTA	5396	N		B 131	77.831	69.542	3.900		
MOTA	5397	CA	TKP	E 131	78.291	70.928	3.865	1.00 29.57	B

MOTA	5398	CB	TRP	E 131	79.538	71.086	2.996	1.00 27.97	_
ATOM	5399			E 131	80.809				E
ATOM	5400			B 131	81.342				B
ATOM	5401				82.551				E
MOTA	5402		3 TRP	E 131	80.913	73.209			E
ATOM	5403		1 TRP		81.689	69.941			E
ATOM	5404		1 TRP		82.738	70.200			E
ATOM	5405			E 131	83.340	72.119			B
ATOM	5406			E 131	81.697	73.900			E
ATOM	5407			E 131	82.900	73.350	6.509	1.00 31.69	E
ATOM	5408	С		E 131	77.185	71.817	3.301	1.00 30.08	E
ATOM	5409	0		B 131	76.449		2.392	1.00 29.15	B
ATOM ATOM	5410	N	PHB		77.081	73.027	3.842	1.00 29.87	E
ATOM	5411	CA		E 132	76.078		3.405	1.00 30.98	E
ATOM	5412 5413	CB		E 132	74.963	74.094	4.443	1.00 32.09	E
ATOM	5414	CG		B 132	74.041	72.918		1.00 33.03	E
ATOM	5415		PHE 2		72.913	72.896		1.00 35.25	E
ATOM	5416		L PHE		74.306	71.822	5.273	1.00 33.31	E
ATOM	5417		2 PHE		72.055	71.794	3.646	1.00 35.49	B
ATOM	5418	CZ		E 132	73.460	70.717	5.279	1.00 35.47	B
ATOM	5419	c		B 132	72.330 76.668	70.704	4.461	1.00 35.97	B
ATOM	5420	ō	PHE		77.537	75.364	3.182	1.00 32.06	E
MOTA	5421	N		E 133	76.186	75.812 76.026	3.929	1.00 29.15	E
ATOM	5422	CA		E 133	76.613	77.375	2.138	1.00 34.68	E
ATOM	5423	CB		E 133	77.281	77.420	1.809 0.434	1.00 37.78	E
MOTA	5424	CG		B 133	77.755	78.810	0.005	1.00 40.14	E
MOTA	5,425	CD		E 133	78.474	78.742	-1.341	1.00 43.27	B
ATOM	5426	NE		E 133	79.096	80.006	-1.738	1.00 46.34 1.00 49.86	B
MOTA	5427	CZ		R 133	78.441	81.058	-2.226	1.00 51.63	B
MOTA	5428	NH1	ARG	E 133	77.124	81.018	-2.387	1.00 51.83	e
ATOM	5429	NH2	ARG	E 133	79.111	82.155	-2.562	1.00 52.46	E
ATOM	5430	C	ARG	E 133	75.343	78.204	1.792	1.00 38.70	B
MOTA	5431	0		E 133	74.569	78.154	0.835	1.00 38.81	E
MOTA	5432	N		B 134	75.119	78.940	2.872	1.00 39.37	E
ATOM	5433	CA		E 134	73.941	79.787	2.984	1.00 42.21	B
ATOM	5434	CB		E 134	74.040	80.952	1.988	1.00 40.37	B
ATOM	5435	CG		B 134	75.383	81.667	2.051	1.00 39.50	B
ATOM	5436		ASN I		75.796	82.151	3.104	1.00 35.36	E
ATOM	5437	ND2			76.071	81.733	0.917	1.00 39.94	E
MOTA	5438	С		3 134	72.652	79.000	2.734	1.00 43.61	B
ATOM ATOM	5439	0	ASN I		71.899	79.306	1.809	1.00 45.62	E
ATOM	5440	N	ASP I		72.403	77.983	3.550	1.00 45.40	E
ATOM	5441 5442	CA C	ASP I		71.189	77.178	3.413	1.00 47.16	E
ATOM	5443	0	ASP B		71.147	76.279	2.173	1.00 48.15	R
ATOM	5444	N	GLN E		70.205	75.504	1.996	1.00 49.25	E
ATOM	5445	CA	GLN E		72.158	76.387	1.316	1.00 48.16	E
ATOM	5446	C	GLN E		72.226 73.254	75.561	0.113	1.00 47.50	E
ATOM	5447	ō	GLN E		74.418	74.445 74.711	0.313	1.00 47.38	E
ATOM	5448	N	GLU E		72.829	73.197	0.627	1.00 46.25	B
MOTA	5449	CA	GLU E		73.749	72.079	0.139	1.00 47.09	E
ATOM	5450	ÇВ	GLU E	137	72.992	70.752	0.308	1.00 47.41 1.00 47.53	E
MOTA	5451	CG	GLU E	137	73.921	69.570	0.653	1.00 49.67	E
MOTA	5452	æ	GLU E		73.210	68.334	1.166	1.00 51.28	e
ATOM	5453	OE1	GLU E	137	73.911	67.336	1.432	1.00 52.31	E
MOTA	5454	OE2	GLU E	137	71.965	68.352	1.306	1.00 51.54	E
MOTA	5455	C	GLU B	137	74.755	72.016	-0.833	1.00 47.37	B
ATOM	5456	0	GLU E	137	74.397	72.163	-2.000	1.00 47.51	E
ATOM	5457	N	GLU E		76.018	71.809	-0.477	1.00 47.53	B
MOTA	5458	CA	GLA E		77.104	71.724	-1.444	1.00 48.48	Ē
MOTA	5459	CB	GLU E		78.266	72.617	-1.011	1.00 49.89	E
ATOM	5460	CG	GLU E		77.949	74.096	-0.973	1.00 54.83	B
MOTA	5461	CD	GLU B		77.911	74.720	-2.354	1.00 57.91	E
MOTA	5462		GLU E		78.953	74.686	-3.044	1.00 59.04	R
MOTA	5463		GLU E		76.846	75.247	-2.748	1.00 58.96	E
MOTA	5464 5465		GLU E		77.593	70.284	-1.532	1.00 48.42	B
MOTA MOTA			GLU E		77.898	69.665	-0.513	1.00 48.62	E
ATOM			THR B		77.665	69.754		1.00 47.87	E
ATOM			THR E		78.135	68.387		1.00 48.16	E
MOTA			THR E		77.027	67.498		1.00 49.05	E
ATOM			THR E		76.464	68.140		1.00 51.25	B
NOT			THR E		75.938	67.249		1.00 48.03	E
•		-			79.339	68.401	-3.895	1.00 46.96	·B

ATOM	5472	0		B 139	80.245	67.574	-3.779	1.00 46.46	B
MOTA	5473	N		E 140	79.339	69.346	-4.827	1.00 46.59	E
ATOM ATOM	5474 5475	CA CB		B 140	80.446	69.488	-5.761	1.00 45.07	E
ATOM	5476	C		E 140 E 140	79.997	70.244	-7.008	1.00 44.64	E
MOTA	5477	Ö		E 140	81.518	70.276	-5.019	1.00 43.57	E
ATOM	5478	N		B 141	81.224 82.756	71.293	-4.386	1.00 43.33	E
ATOM	5479	CA		E 141	83.833	69.805 70.485	-5.091 -4.398	1.00 41.31	E
MOTA	5480	C		B 141	84.053	69.854	-3.034	1.00 38.27 1.00 36.91	E
MOTA	5481	0		E 141	84.930	70.264	-2.272	1.00 37.78	e
ATOM	5482	N	VAL	E 142	83.245	68.849	-2.722	1.00 33.36	E
ATOM	5483	CA		B 142	83.363	68.164	-1.449	1.00 32.16	E
ATOM	5484	CB		B 142	81.978	67.844	-0.847	1.00 31.40	B
ATOM ATOM	5485		VAL		82.140	66.995	0.407	1.00 28.96	E
ATOM	5486		VAL		81.245	69.134	-0.516	1.00 33.20	B
ATOM	5487 5488	C		E 142 E 142	84.140	66.859	-1.576	1.00 31.49	E
ATOM	5489	N		B 143	83.862 85.118	66.032	-2.450	1.00 31.67	B
ATOM	5490	CA		E 143	85.922	66.684 65.473	-0.696	1.00 30.51	E
ATOM	5491	СВ		E 143	87.367	65.731	-0.675 -1.161	1.00 30.35	E
ATOM	5492		VAL		88.096	64.408	-1.348	1.00 30.33	e
MOTA	5493		VAL :		87.347	66.503	-2.460	1.00 33.96	E
MOTA	5494	C	VAL :	B 143	85.966	64.973	0.767	1.00 29.68	E
ATOM	5495	0		E 143	86.242	65.733	1.695	1.00 29.63	E
ATOM	5496	N		B 144	85.696	63.689	0.946	1.00 28.32	E
ATOM	5497	CA		E 144	85.703	63.090	2.268	1.00 25.38	E
ATOM ATOM	5498 5499	CB OG		E 144	84.295	62.613	2.622	1.00 26.70	E
ATOM	5500	C		B 144 E 144	84.300	61.845	3.807	1.00 28.37	E
ATOM	5501	Ö		B 144	86.663 86.824	61.916 61.148	2.361 1.412	1.00 24.56	E
ATOM	5502	N		B 145	87.320	61.790	3.506	1.00 23.42	E
ATOM	5503	CA		B 145	88.218	60.666	3.726	1.00 24.38	e
ATOM	5504	CB		E 145	89.103	60.849	4.983	1.00 24.55	E
ATOM	5505	0 G1			88.273	60.815	6.155	1.00 21.59	B
ATOM	5506		THR I		89.858	62.162	4.935	1.00 24.64	E
MOTA	5507	C		8 145	87.256	59.539	4.055	1.00 23.78	E
ATOM	5508	0		3 145	86.064	59.766	4.242	1.00 23.97	E
ATOM ATOM	5509	N		3 146	87.745	58.300	4.099	1.00 25.25	E
ATOM	5510 5511	CD CA		E 146	88.993	57.713	3.585	1.00 25.42	E
ATOM	5512	CB		3 146	86.770 87.439	57.264 55.983	4.447	1.00 25.00	E
ATOM	5513	CG		3 146	88.905	56.293	3.951 4.094	1.00 26.60 1.00 27.24	E
ATOM	5514	C	PRO E		86.597	57.284	5.976	1.00 27.24	E
ATOM	5515	0	PRO E		87.286	58.030	6.672	1.00 21.73	B
MOTA	5516	N	LEU E	S 147	85.669	56.492	6.495	1.00 23.85	B
MOTA	5517	CA	TEA E		85.476	56.419	7.936	1.00 23.63	B
ATOM	5518	CB	LEU E		84.355	55.428	8.260	1.00 25.11	B
ATOM	5519	CG	LEU E		83.976	55.241	9.731	1.00 28.28	E
ATOM ATOM	5520 5521		LEU E		83.392	56.530	10.270	1.00 29.44	E
ATOM	5521 5522	CD2	TEO E		82.965	54.116	9.867	1.00 28.72	E
ATOM	5523	Ö	LEU E		86.812 87.366	55.915	8.503	1.00 22.77	R
ATOM	5524	N	ILE E		87.337	54.944 56.574	8.003 9.530	1.00 23.04	E
MOTA	5525	CA	ILE E		88.614	56.156	10.102	1.00 19.40	E
ATOM	5526	CB	ILE E		89.588	57.355	10.200	1.00 20.05	E
MOTA	5527	CG2	ILE E		90.903	56.922	10.835	1.00 19.93	E
ATOM	5528		ILE E		89.854	57.918	8.803	1.00 17.58	B
ATOM	5529		ILE E		90.594	59.225	8.821	1.00 20.23	В
ATOM	5530	C	ILE E		. 88.449	55.534	11.489	1.00 17.19 .	E
ATOM	5531	0	ILE E		87.820	56.118	12.360	1.00 15.81	B
ATOM	5532	N	ARG E		89.015	54.344	11.677	1.00 15.23	E
ATOM	5533	CA	ARG E		88.948	53.638	12.956	1.00 16.42	E
MOTA MOTA	5534	CB	ARG E		88.906	52.128	12.724	1.00 20.12	E
ATOM	5535 5536	CD	ARG E		88.903	51.289	14.000	1.00 21.32	E
ATOM	5537	NE	ARG E		88.963 87.825	49.802 49.382	13.649	1.00 22.44	B
ATOM	5538	CZ	ARG E		86.623	49.382	12.830 13.313	1.00 22.55 1.00 22.89	E
ATOM	5539		ARG E		85.650	48.718	12.490	1.00 22.89	B
ATOM	5540		ARG E		86.398	49.139	14.619	1.00 23.36	e
MOTA	5541	С	ARG E		90.174	53.983	13.786	1.00 16.33	B
MOTA	5542	0	ARG E	149	91.305	53.734	13.363	1.00 16.45	B
MOTA	5543	N	asn e		89.953	54.558	14.963	1.00 15.72	8
ATOM	5544	CA	ASN E		91.061	54.948	15.825	1.00 15.93	E
MOTA	5545	CB	asn e	150	90.662	56.125	16.740	1.00 13.37	E

MOTA	5546	œ	asn e	150	90.278	57.383	15.955	1.00 15.55	E
MOTA	5547		asn b		90.922	57.739	14.955	1.00 14.20	E
MOTA	5548		asn b		89.233	58.068	16.414	1.00 15.61	E
MOTA	5549	C	asn b		91.576	53.786	16.670	1.00 16.79	E
MOTA	5550	0	asn e		92.694	53.838	17.180	1.00 18.80	B
ATOM	5551	N	GLY B		90.764	52.745	16.813	1.00 16.63	E
MOTA	5552	CA	GTA E		91.164	51.587	17.593	1.00 18.68	E
MOTA	5553	C	GLY E		90.879	51.684	19.080	1.00 20.19	E
ATOM	5554	0	GLA E		91.087	50.725	19.818	1.00 21.39	E
MOTA	5555	И	ASP E		90.409	52.836	19.539	1.00 19.57	E
MOTA	5556	CA	ASP E		90.108	52.986	20.954	1.00 19.09	E
ATOM	5557	CB	ASP E		90.865	54.177	21.531	1.00 18.53	E
MOTA	5558	CG	ASP E		90.498	55.481	20.856	1.00 21.27 1.00 20.11	e
ATOM	5559		ASP E		89.736 90.984	55.453 56.531	19.864 21.321	1.00 20.11	E
ATOM ATOM	5560 5561	C	ASP E		88.605	53.156	21.182	1.00 19.23	E
ATOM	5562	ō	ASP E		88.177	53.840	22.113	1.00 17.78	13
ATOM	5563	N	TRP E		87.816	52.522	20.318	1.00 18.88	E
ATOM	5564	CA	TRP E		86.356	52.566	20.391	1.00 18.61	B
MOTA	5565	CB	TRP E		85.862	52.162	21.788	1.00 17.06	B
ATOM	5566	CG	TRP E		86.084	50.690	22.085	1.00 17.90	B
MOTA	5567	CD2	TRP E	153	85.165	49.612	21.830	1.00 18.84	R
MOTA	5568	CE2	TRP E	153	85.804	48.414	22.222	1.00 16.88	B
ATOM	5569	CE3	TRP E	153	83.862	49.544	21.308	1.00 18.29	B
MOTA	5570	CD1	TRP E	153	87.209	50.114	22.604	1.00 16.70	B
MOTA	5571	NEl	TRP E	153	87.049	48.747	22.688	1.00 17.49	E
MOTA	5572	CZ2	TRP E	153	85.189	47.164	22.109	1.00 16.54	E
MOTA	5573	CZ3	TRP B	153	83.250	48.303	21.196	1.00 17.19	E
MOTA	5574	CH2	TRP E		83.917	47.129	21.597	1.00 17.24	E
MOTA	5575	C	TRP E		85.732	53.887	19.975	1.00 18.97	E
ATOM	5576	0	TRP E		84.696	54.300	20.508	1.00 18.70	B
MOTA	5577	N	THR E		86.378	54.546	19.016	1.00 19.20	E
ATOM	5578	CA	THR E		85.876	55.794	18.444	1.00 19.92	e
ATOM	5579	CB	THR E		86.442	57.072	19.129	1.00 21.42 1.00 19.26	E
MOTA	5580		THR E		87.865	57.129 57.096	18.958 20.599	1.00 13.20	E
ATOM	5581 5582	CGZ	THR E		86.085 86.314	55.835	16.992	1.00 18.66	E
MOTA MOTA	5583	0	THR E		87.270	55.156	16.603	1.00 19.45	E
ATOM	5584	N	PHE E		85.609	56.626	16.193	1.00 18.54	E
ATOM	5585	CA	PHE E		85.940	56.784	14.779	1.00 19.04	E
MOTA	5586	СВ	PHE I		84.821	56.252	13.882	1.00 20.71	E
ATOM	5587	CG	PHE E		84.524	54.794	14.060	1.00 23.03	B
ATOM	5588		PHE I		83.492	54.375	14.898	1.00 23.94	E
MOTA	5589	CD2	PHE I	E 155	85.255	53.837	13.365	1.00 23.32	B
MOTA	5590	CE1	PHE I	155	83.189	53.017	15.037	1.00 23.82	B
ATOM	5591	CE2	PHE I	3 155	84.962	52.476	13.497	1.00 24.46	B
MOTA	5592	CZ	PHE I	155	83.930	52.068	14.333	1.00 24.51	E
MOTA	5593	C	PHE I		86.109	58.265	14.459	1.00 19.30	B
MOTA	5594	0	PHE I		85.791	59.134	15.275	1.00 19.12	E
ATOM	5595	N	GLN I		86.613	58.550	13.265 12.824	1.00 17.46	E
ATOM	5596	CA	GLN I		86.748	59.924 60.546	13.264	1.00 17.87 1.00 19.74	B
MOTA	5597	CB	GLN I		88.081 89.330	59.948	12.640	1.00 19.80	E
MOTA MOTA	5598 5599	CD		3 156 3 156	90.551	60.785	12.950	1.00 21.46	E
ATOM	5600		GLN I		90.660	61.928	12.503	1.00 21.30	E
ATOM	5601		GLN I		91.469	60.230	13.734	1.00 21.38	E
ATOM	5602	C		E 156	86.629	59.989	11.316	1.00 17.47	B
ATOM	5603	ō		B 156	86.856	58.999	10.616	1.00 17.25	E
MOTA	5604	N		E 157	86.252	61.159	10.823	1.00 17.46	E
MOTA	5605	CA		B 157	86.128	61.363	9.397	1.00 18.92	E
ATOM	5606	CB	ILE I	E 157	84.746	60.922	8.898	1.00 19.57	E
ATOM	5607	CG2	ILE :	E 157	83.659	61.774	9.545	1.00 15.09	B
MOTA	5608	CG1	ILE :	E 157	84.704	60.994	7.369	1.00 21.06	B
MOTA	5609	CD3	ILE	E 157	83.541	60.218	6.756	1.00 22.57	E
ATOM	5610	C	ILE :	E 157	86.349	62.837	9.083	1.00 20.28	B
MOTA	5611	0		B 157	85.887	63.712	9.808	1.00 20.70	B
ATOM	5612	N		E 158	87.094	63.104	8.019	1.00 21.79	E
MOTA	5613	CA		E 158	87.363	64.470	7.601	1.00 23.40	B
MOTA	5614	CB		B 158	88.869	64.706	7.466	1.00 25.42	E
MOTA	5615	CCC		E 158	89.621	65.141 64.154	8.731 9.864	1.00 29.38 1.00 27.98	E
MOTA	5616 5617		LEU		89.384 91.118	65.263	8.412	1.00 27.98	E
MOTA MOTA	5618	CD.	ren 5 Pen	B 158	86.664	64.738	6.271	1.00 23.62	B
ATOM	5619	0		B 158	86.938	64.081	5.264	1.00 22.86	E
M. Ou	2223	•	وعب		55.556				_

ATOM	5620	N	VAL E	159	85.747	65.702	6.290	1.00 22.98	B
MOTA	5621	CA	VAL E	159	84.990	66.087	5.112	1,00 21.37	E
ATOM	5622	СВ	VAL E		83.476	66.104	5.417	1.00 20.53	E
							4.149	1.00 14.20	E
MOTA	5623		VAL E		82.684	66.407			
ATOM	5624	CG2			83.058	64.756	6.002	1.00 15.86	E
MOTA	5625	C	VAL E	159	85.468	67.469	4.710	1.00 22.21	E
MOTA	5626	0	VAL B	159	85.253	68.444	5.423	1.00 22.87	E
ATOM	5627	N	MET E	160	86.116	67.539	3.555	1.00 25.37	E
ATOM	5628	CA	MET E		86.681	68.779	3.049	1.00 27.07	E
						68.494	2.533	1.00 29.57	B
MOTA	5629	CB	MET E		88.088				
MOTA	5630	CG		160	88.996	67.954	3.633	1.00 35.17	E
MOTA	5631	SD	MET E	160	90.519	67.185	3.065	1.00 41.54	E
MOTA	5632	CE	MET E	160	90.011	65.462	2.985	1.00 40.10	B
ATOM	5633	С	MET E	160	85.848	69.466	1.979	1.00 28.93	E
ATOM	5634	ō	MET E		85.191	68.817	1.162	1.00 28.47	B
			TEA B		85.875	70.793	1.997	1.00 29.41	E
MOTA	5635	N						1.00 31.54	B
MOTA	5636	CA	PEO B		85,123	71.574	1.031		
MOTA	5637	CB	LEU B	161	83.931	72.258	1.708	1.00 30.26	E
ATOM	5638	CG	TEO E	161	83.183	73.297	0.860	1.00 30.70	E
MOTA	5639	CD1	LEU B	161	82.515	72.618	-0.332	1.00 29.72	E
ATOM	5640		LEU B		82.145	74.020	1.728	1.00 31.55	E
			LEU B		85.990	72.625	0.363	1.00 32.10	B
MOTA	5641	C						1.00 32.90	B
ATOM	5642	0	PEA B		86.575	73.473	1.029		
MOTA	5643	N	GLU E	162	86.063	72.549	-0.960	1.00 35.11	B
MOTA	5644	CA	GLU E	162	86.820	73.491	-1.771	1.00 38.40	E
ATOM	5645	CB	GLU E	162	87.191	72.838	-3.105	1.00 42.17	B
ATOM	5646	CG	GLU E		87.783	73.776	-4.148	1.00 48.21	B
			GLU E		89.099	74.381	-3.711	1.00 52.47	E
ATOM	5647	CD						1.00 54.02	B
ATOM	5648		Gra B		90.006	73.611	-3.327		
MOTA	5649	OE2	GLU E	162	89.228	75.627	-3.759	1.00 56.21	B
MOTA	5650	C	GLU E	162	85.892	74.673	-2.008	1.00 39.06	E
MOTA	5651	0	GLU E	162	84.750	74.490	-2.422	1.00 39.27	E
MOTA	5652	N	MET E	163	86.369	75.884	-1.747	1.00 40.73	E
			MET E		85.520	77.049	-1.938	1.00 43.18	B
MOTA	5653	CA						1.00 45.15	B
MOTA	5654	CB	WET E		84.546	77.171	-0.761		
MOTA	5655	CG	MET B	163	85.155	76.900	0.612	1.00 47.55	B
MOTA	5656	SD	MET E	163	86.318	78.152	1.185	1.00 52.18	B
MOTA	5657	CB	MET E	163	85.186	79.345	1.941	1.00 50.37	B
ATOM	5658	C	MET E		86.245	78.371	-2.151	1.00 43.77	E
					87.458	78.477	-1.953	1.00 41.87	E
ATOM	5659	0	MET E					1.00 45.83	E
MOTA	5660	N	THR E		85.474	79.371	-2.571		
ATOM	5661	CA	THR E	164	85.981	80.714	-2.827	1.00 49.20	E
MOTA	5662	CB	THR E	164	85.585	81.177	-4.241	1.00 50.11	Ē
ATOM	5663	OG1	THR E	164	86.036	80.208	-5.199	1.00 49.28	E
ATOM	5664	CG2	THR E	164	86.204	82.535	-4.559	1.00 50.19	B
ATOM	5665	C	THR E		85.371	81.652	-1.785	1.00 51.14	E
			THR E		84.169	81.916	-1.802	1.00 50.64	E
MOTA	5666	0					-0.864	1.00 53.75	B
ATOM	5667	N	PRO E		86.198	82.170			Ē
MOTA	5668	CD	PRO E	165	87.667	82.057	-0.818	1.00 54.65	
ATOM	5669	CA	PRO E	165	85.719	83.072	0.185	1.00 56.16	E
ATOM	5670	CB	PRO E	165	86.965	83.299	1.036	1.00 55.47	B
ATOM	5671	CG	PRO F	165	88.057	83.262	0.019	1.00 55.93	B
ATOM	5672	C	PRO I	3 165	85.098	84.381	-0.291	1.00 58.83	E
	5673		PRO I		85.673	85.100	-1.112	1.00 58.35	E
ATOM		0	GIN I		83.912	84.666	0.239	1.00 61.77	E
MOTA	5674	N						1.00 63.96	E
ATOM	5675	CA	GLN I		83.173	85.885	-0.065		
MOTA	5676	CB	GLN I	Z 166	82.103	85.616	-1.123	1.00 64.28	E
MOTA	5677	CG	GLN I	3 166	82.662	85.236	-2.481	1.00 66.42	B
MOTA	5678	CD	GLN I	E 166	81.643	85,392	-3.596	1.00 67.38	E
MOTA	5679		C GLM	E 166	81.937	85.124	-4.761	1.00 68.28	; E
ATOM			GLN I		80.437	85.832	-3.244	1.00 66.50	E
	5680			B 166	82.521		1.223	1.00 65.40	B
MOTA	5681	C							E
MOTA	5682	0		E 166	81.974		2.007	1.00 65.65	
ATOM	5683	N		B 167	82.589		1.444	1.00 65.80	E
MOTA	5684	CA	ARG :	B 167	82.017	88.302	2.647	1.00 65.27	B
MOTA	5685	CB	ARG	E 167	82.353	89.795	2.706	1.00 67.87	E
ATOM	5686	CG		B 167	82.221		4.095	1.00 70.91	E
				E 167	83.216		5.085	1.00 73.36	B
ATOM	5687	CD						1.00 75.19	E
MOTA	5688	NE		B 167	83.244		6.359		E
ATOM	5689	CZ		B 167	84.012		7.394	1.00 75.48	
MOTA	5690		1 ARG		84.824		7.318	1.00 75.50	E
MOTA	5691	NH	2 ARG	R 167	83.968	90.916	8.509	1.00 75.83	E
ATOM	5692		ARG	E 167	80.504	88.100	2.684	1.00 63.81	E
ATOM	5693			B 167	79.816		1.672	1.00 62.94	E
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MOTA	5694	N	GLY I	3 16	79.991	87.751	3.860	1.00 61.88	E
MOTA	5695	CA	GLY I	B 16	78.567	87.519	4.004	1.00 58.78	E
ATOM	5696	C	GLY I			86.036	3.959	1.00 57.24	E
			GLY !						Б
MOTA	5697	0				85.594	4.558	1.00 57.26	
MOTA	5698	N	ASP I			85.263	3.249	1.00 54.67	E
MOTA	5699	CA	ASP I	E 16	78.849	83.823	3.140	1.00 52.07	E
MOTA	5700	CB	ASP :	B 16	79.799	83.186	2.116	1.00 52.03	E
ATOM	5701	CG	ASP 1				0.683	1.00 52.57	E
ATOM	5702		ASP 1				0.457	1.00 51.86	B
MOTA	5703		ASP 1				-0.223	1.00 52.34	B
MOTA	5704	C	ASP I	B 16	79.027	83.096	4.463	1.00 49.54	E
MOTA	5705	0	ASP :	E 16	79.993	83.322	5.196	1.00 49.84	E
MOTA	5706	N	VAL 1	E 17	78.082	82.214	4.758	1.00 46.54	E
ATOM	5707	CA	VAL I				5.970	1.00 43.15	B
			VAL				6.871	1.00 42.70	E
ATOM	5708	CB							
MOTA	5709		VAL :				8.138	1.00 41.36	E
MOTA	5710	CG2	VAL :	B 17	76.814	83.146	7.227	1.00 41.14	E
MOTA	5711	С	VAL	E 17	78.172	79.948	5.555	1.00 41.66	B
MOTA	5712	0	VAL :	E 17	77.216	79.432	4.972	1.00 40.25	E
ATOM	5713	N	TYR				5.833	1.00 39.16	B
							5.502	1.00 38.16	B
ATOM	5714	CA	TYR						
MOTA	5715	CB	TYR				4.953	1.00 38.66	B
MOTA	5716	CG	TYR	E 17	. 81.035	78.237	3.598	1.00 38.98	B
ATOM	5717	CD1	TYR	B 17	80.740	77.522	2.440	1.00 38.79	B
ATOM	5718	CKI	TYR	B 17	80.852	78.105	1.186	1.00 40.42	B
ATOM	5719		TYR				3.471	1.00 38.62	E
								1.00 40.32	B
ATOM	5720		TYR				2.219		
ATOM	5721	CZ	TYR			79.424	1.079	1.00 41.26	B
MOTA	5722	OH	TYR	E 17	. 81.350	80.004	-0.166	1.00 42.98	B
MOTA	5723	C	TYR	B 17	. 79.206	77.076	6.764	1.00 37.15	B
ATOM	5724	o	TYR	R 17			7.813	1.00 37.94	E
	5725	N	THR				6.672	1.00 35.12	E
MOTA								•	E
ATOM	5726	CA	THR				7.842	1.00 34.42	
ATOM	5727	CB	THR			75.496	8.367	1.00 35.21	E
MOTA	5728	OG1	THR	E 17	76.184	74.351	9.094	1.00 35.96	E
MOTA	5729	CG2	THR	E 17	75.706	75.790	7.226	1.00 38.35	E
MOTA	5730	C	THR			73.734	7.638	1.00 32.90	B
			THR				6.604	1.00 31.57	E
MOTA	5731	0							В
MOTA	5732	N	CYS				8.643	1.00 30.59	
MOTA	5733	CA	CYS				8.640	1.00 29.35	E
MOTA	5734	С	CYS	E 17	77.923	71.058	9.454	1.00 29.72	E
ATOM	5735	0	CYS	E 17	3 77.771	71.337	10.645	1.00 28.89	E
ATOM	5736	CB	CYS	E 17	80.424	71.299	9.287	1.00 27.53	E
MOTA	5737	SG	CYS				9.133	1.00 27.81	E
							8.788	1.00 28.95	E
MOTA	5738	N	HIS						
MOTA	5739	CA	HIS				9.381	1.00 28.54	E
MOTA	5740	CB	HIS	B 17	1 74.770	69.881	8.399	1.00 29.66	B
ATOM	5741	CG	HIS	E 17	73.457	69.311	8.823	1.00 30.98	E
ATOM	5742	CD2	HIS	B 17	72.367	69.899	9.369	1.00 31.91	R
ATOM	5743		HIS			67.988	8.630	1.00 31.68	H
ATOM	5744		HIS				9.034	1.00 33.26	B
									E
MOTA	5745		HIS				9.487	1.00 34.66	
ATOM	5746	C	HIS				9.650	1.00 27.83	E
MOTA	5747	0	HIS	E 17	4 76.438	67.375	8.728	1.00 27.35	B
ATOM	5748	N	VAL	B 17	5 76.085	67.753	10.917	1.00 26.27	E
ATOM	5749	CA	VAL	E 17	5 76.349	66.365	11.284	1.00 26.34	B
MOTA	5750	СВ		E 17			12.215	1.00 23.90	B
			VAL				12.663	1.00 19.67	B
ATOM	5751						11.491	1.00 19.93	B
MOTA	5752		VAL						
MOTA	5753	C	VAL	E 1			11.938	1.00 27.67	E
MOTA	5754	0	VAL	E 1	5 74.587	7 66.064	12.904	1.00 26.77	E
MOTA	5755	N	GLU	B 1'	6 74.917	7 64.423	11.399	1.00 29.83	E
MOTA	5756	CA		E 1			11.929	1.00 32.99	E
ATOM	5757	СВ		E 1			10.839	1.00 34.86	E
								1.00 40.13	E
ATOM	5758	CG		E 1			10.319		
MOTA	5759	æ		E J.			9.124	1.00 44.38	E
MOTA	5760	OE:	L GILT	E 1	6 70.292	2 63.265	9.269	1.00 46.31	B
MOTA	5761	OE:	GLU	E 1	6 71.433	64.682	8.037	1.00 47.49	E
MOTA	5762	C		E 1			12.445	1.00 32.24	B
ATOM	5763	ō		E 1			11.734	1.00 32.81	E
							13.686	1.00 31.66	E
ATOM	5764	N		E 1					E
MOTA	5765	CA		E 1			14.311	1.00 30.50	
ATOM	5766	CB		E 1			14.927	1.00 29.59	E
ATOM	5767	CG	HIS	E 1	7 76.87	1 60.034	15.582	1.00 28.23	В

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MOTA	5768		HIS			77.752	59.134	15.086		28.22	B
MOTA	5769	ND1	HIS	E	177	76.679	59.698	16.903	1.00	27.71	B
ATOM	5770	CE1	HIS	E	177	77.410	58.636	17.194	1.00	29.83	B
MOTA	5771	NE2	HIS	E	177	78.070	58.274	16.108		29.78	B
MOTA	5772	C	HIS			73.854	60.195	15.373		30.09	E
MOTA	5773	0	HIS	ĸ	177	73.189	60.942	16.083	1.00	29.91	B
MOTA	5774	N	PRO	E	178	73.781	58.862	15.496	1.00	31.45	B
MOTA	5775	æ	PRO	E	178	74.485	57.842	14.697	1.00	31.00	E
ATOM	5776	CA	PRO			72.898	58.226				
								16.481		31.44	R
MOTA	5777	CB	PRO	E	178	73.370	56.779	16.467	1.00	30.89	B
ATOM	5778	CG	PRO	E	178	73.704	56.578	15.028	1.00	31.16	E
ATOM	5779	C	PRO	Е	178	72.896	58.826	17.893	1.00	31.78	B
ATOM	5780	ō	PRO			71.903	58.727	18.611		32.84	B
ATOM	5781	N	SER			73.996	59.448	18.292	1.00	30.31	B
ATOM	5782	CA	SER	B	179	74.087	60.039	19.624	1.00	30.84	B
MOTA	5783	CB	SER	E	179	75.552	60.155	20.038	1.00	29.11	B
ATOM	5784	OG	SER			76.240	61.049	19.176		24.79	E
MOTA	5785	С	SER			73.452	61.424	19.717		32.75	B
MOTA	5786	0	SER	E	179	73.330	61.982	20.804	1.00	32.78	B
ATOM	5787	N	LEU	B	180	73.046	61.981	18.583	1.00	35.18	E
ATOM	5788	CA	LEU			72.477	63.317	18.578		37.31	E
MOTA	5789	CB	LEU			73.098	64.132	17.448		35.77	E
ATOM	5790	CG	LEU	E	180	74.610	64.337	17.528	1.00	36.46	E
ATOM	5791	CD1	LEO	B	180	75.097	65.018	16.259	1.00	35.16	B
MOTA	5792	CD2	LEU	R	180	74.948	65.167	18.752		34.58	E
ATOM	5793	C	LEU			70.967	63.405	18.463		40.35	E
MOTA	5794	0	PEA	E	180	70.386	63.003	17.456	1.00	40.67	E
MOTA	5795	N	GLN	E	181	70.338	63.943	19.503	1.00	42.97	E
MOTA	5796	CA	GLN	R	181	68.895	64.141	19.504	1.00	45.09	E
MOTA	5797	CB	GLN			68.466	64.877	20.776		46.73	E
MOTA	5798	CG	GTN	E	181	69.471	65.931	21.235	1.00	49.84	E
MOTA	5799	CD	GLN	E	181	68.898	66.904	22.256	1.00	52.17	E
MOTA	5800	ORI	GLN	R	181	68.074	67.760	21.920	1.00	52.91	E
ATOM	5801	NE2				69.329	66.774	23.510		51.73	E
MOTA	5802	C	GLW			68.607	65.002	18.277		45.26	B
MOTA	5803	0	GLN	В	181	67.660	64.752	17.530	1.00	46.25	E
ATOM	5804	N	SER	E	182	69.448	66.013	18.078	1.00	44.33	В
MOTA	5805	CA			182	69.335	66.923	16.943	1.00	42.52	E
											E
MOTA	5806	СВ			182	68.819	68.291	17.401		43.41	
MOTA	5807	OG	SER	E	182	69.658	68.853	18.396	1.00	43.07	E
MOTA	5808	C	SER	B	182	70.725	67.068	16.337	1.00	41.70	E
ATOM	5809	0	SER	R	182	71.726	66.955	17.040	1.00	39.94	B
						70.805	67.330	15.023		41.57	E
MOTA	5810	N			183						
MOTA	5811	CD	PRO	Е	183	69.680	67.554	14.098	1.00	41.72	B
ATOM	5812	CA	PRO	B	183	72.087	67.485	14.326	1.00	40.68	E
MOTA	5813	CB	PRO	E	183	71.669	67.638	12.865	1.00	40.95	B
MOTA	5814	CG			183	70.344	68.309	12.965		42.76	E
ATOM	5815	Ç			183	72.988	68.628	14.790		38.81	E
ATOM	5816	0	PRO	E	183	72.520	69.709	15.142	1.00	39.64	B
MOTA	5817	N	ILE	E	184	74.291	68.370	14.785	1.00	37.31	E
MOTA	5818	CA	ILE	R	184	75,270	69.368	15.177	1.00	34.30	E
ATOM	5819	СВ			184	76.570	68.728	15.699		33.43	E
MOTA	5820		ILE			77.671	69.779	15.766		32.87	E
ATOM	5821	CG1	ILE	Е	184	76.337	68.112	17.076	1.00	33.53	B
MOTA	5822	CD1	ILE	E	184	77.530	67.339	17.604	1.00	33.29	E
MOTA	5823	C			184	75.625	70.216	13.974	1.00	33.68	E
										33.87	E
MOTA	5824	0			184	75.851	69.704	12.882			
MOTA	5825	N	THR	E	185	75.676	71.521	14.181		34.19	E
MOTA	5826	CA	THR	E	185	76.018	72.431	13.111	1.00	33.39	E
MOTA	5827	CB	THR	E	185	74.792	73.230	12.637	1.00	33.77	B
			THR			74.211	73.918	13.751		33.46	E
ATOM	5828										
ATOM	5829		THR			73.758	72.297	12.016		33.35	E
MOTA	5830	C	THR	E	185	77.081	73.396	13.590	1.00	33.01	B
ATOM	5831	0			185	76.990	73.966	14.679	1,00	33.25	B
ATOM	5832	N			186	78.106	73.552	12.770		32.85	B
							74.453	13.067		32.84	B
ATOM	5833	CA			186	79.197					
MOTA	5834	CB			186	80.503	73.684	13.300		31.58	E
MOTA	5835	CG1	VAL	E	186	81.629	74.651	13.611	1.00	30.07	B
MOTA	5836	CG2	VAL	В	186	80.316	72.697	14.441	1.00	30.84	B
ATOM	5837	c			186	79.329	75.317	11.836		34.14	B
						79.403				33.50	B
MOTA	5838	0			186		74.812	10.719			
MOTA	5839	N			187	79.329	76.626	12.029		38.05	B
MOTA	5840	CA	GLU	B	187	79.453	77.522	10.898	1.00	40.60	E
ATOM	5841	СВ			187	78.358	78.592	10.934	1.00	43.36	E
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NAME	ATOM	5842	CG	GLU	B	187	78.426	79.531	12.121	1.00 47.46	B
NETON SA64 CRE C GLU E 187	MOTA	5843	CD				77.657	80.822	11.886	1.00 51.49	
AROM S846 C GLU E 187 80.819 78.162 10.077 1.00 40.49 E RATOM S847 0 GLU E 187 81.496 78.265 11.901 1.00 40.26 E RATOM S849 N TRP E 188 81.221 78.610 9.668 1.00 41.52 E RATOM S850 CB TRP E 188 83.498 78.337 81.00 41.52 E RATOM S850 CB TRP E 188 83.498 78.337 81.00 41.52 E RATOM S851 CG TRP E 188 88.492 78.942 8.675 1.00 41.34 E RATOM S851 CG TRP E 188 88.492 78.942 8.675 1.00 41.34 E RATOM S851 CB TRP E 188 88.527 79.672 79.672 1.00 40.23 E RATOM S855 CD1 TRP E 188 88.297 79.672 79.672 70.00 1.00 41.34 E RATOM S855 CD1 TRP E 188 86.642 80.005 7.838 1.00 41.07 E RATOM S855 CD1 TRP E 188 86.642 80.005 78.801 1.00 41.07 E RATOM S855 CD1 TRP E 188 86.642 80.005 78.801 1.00 41.09 E RATOM S855 CD1 TRP E 188 86.67 78.945 9.588 1.00 41.09 41.99 E RATOM S855 CD1 TRP E 188 86.947 79.622 9.003 1.00 41.99 E RATOM S855 CD1 TRP E 188 86.947 79.622 9.003 1.00 41.99 E RATOM S855 CD1 TRP E 188 86.947 79.622 9.003 1.00 41.99 E RATOM S856 CD1 TRP E 188 86.947 19.622 9.003 1.00 41.99 E RATOM S856 CD1 TRP E 188 86.947 19.622 9.003 1.00 41.99 E RATOM S856 CD1 TRP E 188 86.947 19.622 9.003 1.00 42.58 E RATOM S856 CD1 TRP E 188 86.947 19.622 9.003 1.00 42.58 E RATOM S856 CD1 TRP E 188 86.947 19.622 9.003 1.00 42.58 E RATOM S856 CD1 TRP E 188 86.947 19.622 9.003 1.00 42.58 E RATOM S856 CD1 TRP E 188 86.947 19.604 19.505 0.004 19.90 E RATOM S856 CD1 TRP E 188 86.949 19.505 0.004 19.90 E RATOM S856 CD1 TRP E 188 86.949 19.505 0.004 19.90 E RATOM S856 CD1 TRP E 188 86.949 19.505 0.004 19.90 E RATOM S856 CD1 TRP E 188 86.949 19.505 0.004 19.90 E RATOM S856 CD1 TRP E 188 86.949 19.505 0.004 19.90 E RATOM S856 CD1 TRP E 188 86.949 19.505 0.004 19.90 E RATOM S856 CD1 TRP E 188 86.949 19.505 0.004 19.90 E RATOM S856 CD1 TRP E 188 86.949 19.505 0.004 19.90 E RATOM S856 CD1 TRP E 188 86.949 19.505 0.004 19.90 E RATOM S856 CD1 TRP E 188 86.949 19.505 0.004 19.90 E RATOM S856 CD1 TRP E 188 86.949 19.505 0.004 19.90 E RATOM S856 CD1 TRP E 188 86.949 19.505 0.004 19.90 E RATOM S856 CD1 TRP E 189 88.505 0.004 19.90 E RATOM S856 CD1 TRP E 189 88.505 0	ATOM	5844	OB1	GLU	E	187	76.452	80.752	11.551	1.00 52.89	В
NATION SAME Name 188 18.496 78.285 11.901 1.00 40.26 E	ATOM	5845	OE2	GLU :	E	187	78.262	81.908	12.039	1.00 53.48	E
NATION SAME N TRUE 188	MOTA	5846	C	GLU	E	187	80.819	78.182	10.877	1.00 40.49	B
NATION SASS CA TRUE E 188 82.492 79.284 9.488 1.00 43.59 E		5847	0	GLU	E	187	81.496	78.285	11.901	1.00 40.26	B
NATION SSS5 CG		5848	И								
NATION SSS1											
XTOMN S852 CDZ TRP E 188 85.327 79.672 7.543 1.00 40.23 E XTOMN S854 CBZ TRP E 188 86.642 80.090 7.83 1.00 41.87 E XTOMN S855 CDI TRP E 188 86.642 80.015 6.305 1.00 40.90 E XTOMN S855 CDI TRP E 188 86.867 78.945 9.588 1.00 41.89 E XTOMN S857 CBZ TRP E 188 86.867 78.945 9.588 1.00 41.89 E XTOMN S857 CBZ TRP E 188 86.837 79.612 9.093 1.00 41.89 E XTOMN S858 CBZ TRP E 188 86.837 87.411 80.835 6.938 1.00 42.93 E XTOMN S859 CBZ TRP E 188 86.839 81.159 5.731 1.00 43.65 E XTOMN S859 CBZ TRP E 188 86.839 81.159 5.731 1.00 43.65 E XTOMN S850 C TRP E 188 86.839 81.159 5.731 1.00 43.65 E XTOMN S851 O TRP E 188 86.839 81.159 5.731 1.00 43.65 E XTOMN S851 O TRP E 188 81.335 80.374 7.688 1.00 42.53 E XTOMN S852 CN ARG E 189 82.998 81.579 8.765 1.00 50.26 E XTOMN S856 CD ARG E 189 82.673 82.761 7.936 1.00 54.31 E XTOMN S856 CD ARG E 189 82.673 82.761 7.936 1.00 54.31 E XTOMN S856 CD ARG E 189 83.580 84.460 9.880 1.00 59.58 E XTOMN S856 CD ARG E 189 83.590 84.460 9.880 1.00 66.73 E XTOMN S856 CD ARG E 189 83.590 84.791 12.215 1.00 66.73 E XTOMN S857 NEL ARG E 189 83.590 84.791 12.215 1.00 66.73 E XTOMN S857 NEL ARG E 189 85.573 84.796 13.363 1.00 67.41 E XTOMN S870 NEL ARG E 189 85.573 84.766 13.363 1.00 67.41 E XTOMN S870 NEL ARG E 189 85.573 84.766 1.00 55.74 E XTOMN S870 NEL ARG E 189 85.573 84.766 1.00 55.74 E XTOMN S870 NEL ARG E 189 85.573 84.766 1.00 56.16 E XTOMN S870 NEL ARG E 189 85.573 84.766 1.00 56.16 E XTOMN S870 NEL ARG E 189 85.573 84.766 1.00 56.16 E XTOMN S870 NEL ARG E 189 85.573 84.766 1.00 56.16 E XTOMN S870 NEL ARG E 189 85.573 84.766 1.00 56.74 E XTOMN S870 NEL ARG E 189 85.573 84.766 1.00 56.74 E XTOMN S870 NEL ARG E 189 85.573 84.766 1.00 56.74 E XTOMN S870 NEL ARG E 189 85.573 84.766 1.00 56.74 E XTOMN S870 NEL ARG E 189 85.573 84.766 1.00 56.74 E XTOMN S870 NEL ARG E 189 85.573 84.766 1.00 56.74 E XTOMN S870 NEL ARG E 189 85.573 84.766 1.00 56.74 E XTOMN S870 NEL ARG E 189 85.573 84.766 1.00 56.74 E XTOMN S870 NEL ARG E 189 85.7											
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ATOM											
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ATOM											
ATOM 5866 CB ARG E 189 81.980 83.855 8.755 1.00 56.19 8 ATOM 5866 CD ARG E 189 82.820 84.460 9.880 1.00 59.58 E ATOM 5866 CD ARG E 189 83.030 83.499 11.045 1.00 63.51 E ATOM 5866 CZ ARG E 189 83.580 84.180 12.218 1.00 66.73 E ATOM 5869 NH1 ARG E 189 84.771 84.771 12.255 1.00 68.44 E ATOM 5869 NH1 ARG E 189 85.573 84.766 11.183 1.00 69.41 E ATOM 5870 NH2 ARG E 189 85.573 84.766 11.183 1.00 59.41 E ATOM 5871 C ARG E 189 85.573 84.766 11.183 1.00 55.74 E ATOM 5873 N ALA E 190 85.583 84.786 61.56 1.00 56.16 E ATOM 5873 N ALA E 190 84.920 84.557 5.435 1.00 55.74 E ATOM 5875 CB ALA E 190 84.920 84.957 83.964 10.00 55.77 E ATOM 5876 CC ALA E 190 84.520 84.734 3.964 1.00 59.97 E ATOM 5876 C ALA E 190 84.520 84.557 5.435 1.00 60.08 E ATOM 5877 O ALA E 190 86.538 86.479 5.558 1.00 61.01 E ATOM 5878 OXT ALA E 190 86.538 86.479 5.558 1.00 61.05 E ATOM 5878 OXT ALA E 190 86.534 86.378 6.971 1.00 62.25 E ATOM 5880 O LEU F 1 78.718 38.094 33.366 1.00 32.03 F ATOM 5881 N LEU F 1 78.718 38.094 33.366 1.00 32.03 F ATOM 5882 CA LEU F 1 77.422 38.678 33.658 1.00 32.79 F ATOM 5883 N GLN F 2 78.678 37.069 32.531 1.00 32.59 F ATOM 5883 N GLN F 2 78.678 37.069 32.531 1.00 32.59 F ATOM 5883 C GLN F 2 79.649 36.031 31.935 1.00 32.59 F ATOM 5883 C G LIF F 1 78.744 36.436 31.936 1.00 32.79 F ATOM 5888 C G GN F 3 80.465 36.666 1.00 32.79 F ATOM 5888 C G FOF F 3 80.466 36.679 32.531 1.00 32.59 F ATOM 5889 C G FOF F 3 80.466 36.666 1.00 27.93 F ATOM 5890 C B FOF F 3 80.466 37.069 32.531 1.00 30.39 F ATOM 5890 C B FOF F 3 80.466 37.069 32.531 1.00 30.39 F ATOM 5890 C B FOF F 3 80.466 37.069 32.531 1.00 28.02 F ATOM 5890 C B FOF F 3 80.467 37.069 32.531 1.00 27.68 F ATOM 5890 C B FOF F 3 80.467 37.069 32.531 1.00 27.68 F ATOM 5890 C B FOF F 3 80.467 37.069 32.531 1.00 27.68 F ATOM 5890 C B FOF F 3 80.467 37.069 32.531 1.00 27.18 F ATOM 5890 C B FOF F 3 80.479 37.369 37.398 1.00 27.18 F ATOM 5890 C B FOF F 3 80.479 37.399 37.390 1.00 27.18 F ATOM 5890 C C FOF F 3 80.479 37.390 37.390 1.00 27.18 F ATOM 5890 C C FOF F 5 80.499 37.390 37.390 1.00									7.936	1.00 54.31	E
ATOM 5866 CD ARG E 189 83.030 83.499 11.045 1.00 63.51 E ATOM 5867 NB ARG E 189 83.580 84.781 12.218 1.00 66.73 E ATOM 5868 CZ ARG E 189 84.771 84.771 12.255 1.00 69.41 E ATOM 5869 NH1 ARG E 189 85.553 84.766 11.183 1.00 69.41 E ATOM 5870 NH2 ARG E 189 85.573 84.766 11.183 1.00 59.41 E ATOM 5871 C ARG E 189 85.178 65.378 13.363 1.00 70.13 E ATOM 5871 C ARG E 189 85.178 65.378 13.363 1.00 55.74 E ATOM 5873 N ALA E 190 84.920 84.557 5.435 1.00 55.16 E ATOM 5873 N ALA E 190 84.920 84.557 5.435 1.00 60.08 E ATOM 5875 CB ALA E 190 84.920 84.557 5.435 1.00 60.08 E ATOM 5876 C ALA E 190 84.554 86.378 6.971 1.00 62.25 E ATOM 5876 O ALA E 190 84.654 86.378 6.971 1.00 62.25 E ATOM 5876 O ALA E 190 86.338 86.479 5.558 1.00 61.05 E ATOM 5879 C LEU F 1 79.818 38.578 33.365 1.00 61.01 E ATOM 5879 C LEU F 1 79.818 38.578 33.365 1.00 30.77 F ATOM 5881 N LEU F 1 79.818 38.578 33.365 1.00 32.03 F ATOM 5882 CA LEU F 1 77.422 38.678 33.953 1.00 32.25 F ATOM 5882 CA LEU F 1 77.422 38.678 33.953 1.00 33.21 F ATOM 5882 CA LEU F 1 77.422 38.678 33.953 1.00 33.21 F ATOM 5885 C GLN F 2 78.578 77.069 36.081 30.462 1.00 27.93 F ATOM 5885 C GLN F 2 79.609 36.081 30.462 1.00 27.93 F ATOM 5885 C GLN F 2 79.609 36.081 30.462 1.00 27.93 F ATOM 5885 C GLN F 2 79.609 36.081 30.462 1.00 27.76 F ATOM 5885 C GLN F 2 79.744 36.432 31.936 1.00 33.21 F ATOM 5886 C G GLN F 2 79.744 36.432 31.936 1.00 27.76 F ATOM 5895 C G PRO F 3 80.463 37.575 88.660 1.00 28.84 F ATOM 5895 C G PRO F 3 80.463 37.595 86.600 1.00 28.61 F ATOM 5895 C G PRO F 3 80.463 37.595 86.600 1.00 28.61 F ATOM 5895 C G PRO F 3 80.463 37.595 86.600 1.00 28.02 F ATOM 5895 C G PRO F 3 80.463 37.595 86.600 1.00 28.02 F ATOM 5895 C G PRO F 3 80.463 37.595 86.600 1.00 28.41 F ATOM 5895 C G PRO F 3 80.463 37.595 86.600 1.00 28.41 F ATOM 5895 C G PRO F 3 80.463 37.595 86.600 1.00 28.41 F ATOM 5895 C G PRO F 3 80.463 37.595 86.600 1.00 28.41 F ATOM 5895 C G PRO F 3 80.473 31.480 22.535 1.00 31.89 F ATOM 5895 C G PRO F 5 80.484 79.745 22.500 22.505 F ATOM 5895 C G PRO F 5 80.484 79.524 27.999 2			CB	ARG	B	189	81.980	83.855	8.755	1.00 56.19	B
ATOM 5866 NE ARG E 189 83.580 84.180 12.218 1.00 66.73 E ATOM 5869 NH1 ARG E 189 85.553 84.766 11.283 1.00 68.44 E ATOM 5869 NH1 ARG E 189 85.578 85.578 13.363 1.00 70.13 E ATOM 5870 NH2 ARG E 189 85.578 83.722 7.313 1.00 56.16 E ATOM 5871 C ARG E 189 83.950 83.322 7.313 1.00 56.16 E ATOM 5872 O ARG E 189 83.950 83.322 7.313 1.00 56.16 E ATOM 5873 N ALA E 190 83.796 83.962 6.156 1.00 56.16 E ATOM 5874 CA ALA E 190 84.520 84.577 5.435 1.00 60.08 E ATOM 5875 CB ALA E 190 84.550 84.734 3.964 1.00 59.97 E ATOM 5876 C ALA E 190 84.550 84.734 3.964 1.00 59.97 E ATOM 5876 C ALA E 190 84.550 84.734 3.964 1.00 59.97 E ATOM 5877 O ALA E 190 86.338 86.378 6.378 1.00 62.25 E ATOM 5879 C LEU F 1 79.818 38.054 33.366 1.00 61.85 E ATOM 5879 C LEU F 1 79.818 38.054 33.366 1.00 30.77 F ATOM 5880 C LEU F 1 79.818 38.571 33.568 1.00 30.77 F ATOM 5881 N LEU F 1 77.422 38.100 33.307 1.00 33.21 F ATOM 5884 CA GLN F 2 79.444 36.436 31.936 1.00 32.59 F ATOM 5884 CA GLN F 2 79.609 36.081 33.307 1.00 32.59 F ATOM 5885 C GLN F 2 79.609 36.081 30.062 1.00 27.93 F ATOM 5886 C GLN F 2 79.609 36.081 30.062 1.00 27.93 F ATOM 5889 CA FRO F 3 80.463 36.663 29.619 1.00 28.02 F ATOM 5889 CA FRO F 3 80.463 36.665 29.450 1.00 27.76 F ATOM 5889 CA FRO F 3 80.463 36.665 29.450 1.00 27.76 F ATOM 5889 CA FRO F 3 80.463 36.665 29.450 1.00 27.76 F ATOM 5889 CA FRO F 3 80.463 36.665 29.450 1.00 28.02 F ATOM 5889 CA FRO F 3 80.463 36.665 29.450 1.00 28.02 F ATOM 5899 CD FRO F 3 80.463 37.298 27.552 1.00 28.01 F ATOM 5899 CD FRO F 3 80.463 37.298 27.552 1.00 28.01 F ATOM 5899 CD FRO F 3 80.463 37.298 27.552 1.00 28.01 F ATOM 5899 CD FRO F 3 80.479 30.533 37.598 27.552 1.00 28.01 F ATOM 5899 CD FRO F 3 80.479 30.539 27.466 1.00 24.75 F ATOM 5899 CD FRO F 3 80.479 30.539 27.466 1.00 24.75 F ATOM 5899 CD FRO F 3 80.479 30.539 27.466 1.00 24.75 F ATOM 5899 CD FRO F 5 80.489 30.490 27.446 1.00 27.24 F ATOM 5890 CD FRO F 5 80.489 30.490 27.446 1.00 27.24 F ATOM 5890 CD FRO F 5 80.489 30.490 27.446 1.00 20.29 F ATOM 5890 CD FRO F 5 80.489 30.490 27.446 1.00 20.29	ATOM	5865	CG	ARG	B	189	82.820	84.460	9.880	1.00 59.58	B
ATOM 5869 CZ ARG E 189 84.771 84.771 12.255 1.00 68.44 E ATOM 5869 NH1 ARG E 189 85.553 84.766 11.183 1.00 69.41 E ATOM 5870 NH2 ARG E 189 85.553 85.578 13.363 1.00 70.13 E ATOM 5871 C ARG E 189 83.950 83.322 7.313 1.00 55.74 E ATOM 5872 C ARG E 189 83.950 83.322 7.361 1.00 55.74 E ATOM 5873 N ALA E 190 83.796 83.962 6.156 1.00 56.16 E ATOM 5874 CA ALA E 190 84.550 84.734 3.964 1.00 59.97 E ATOM 5875 CB ALA E 190 84.550 84.734 3.964 1.00 59.97 E ATOM 5876 C ALA E 190 84.654 86.378 6.971 1.00 60.08 E ATOM 5877 O ALA E 190 84.654 86.378 6.971 1.00 62.25 E ATOM 5878 OX ALA E 190 86.338 86.479 5.558 1.00 61.01 E ATOM 5878 OX ALA E 190 86.338 86.479 5.558 1.00 61.01 E ATOM 5878 OX ALA E 190 86.338 86.479 5.558 1.00 61.01 E ATOM 5878 OX ALA E 190 86.338 86.479 5.558 1.00 61.05 E ATOM 5878 OX ALA E 190 86.338 86.479 5.558 1.00 61.05 E ATOM 5878 OX EUF 1 78.718 38.094 33.366 1.00 32.03 F ATOM 5880 O LEU F 1 78.718 38.094 33.366 1.00 32.03 F ATOM 5881 N LEU F 1 76.219 38.100 33.070 1.00 33.21 F ATOM 5882 CA LEU F 1 77.432 38.100 33.070 1.00 33.21 F ATOM 5884 CA GLIN F 2 78.578 37.069 32.551 1.00 33.25 F ATOM 5886 CO GLIN F 2 79.640 36.436 31.936 1.00 28.84 F ATOM 5886 CO GLIN F 2 79.640 36.643 31.936 1.00 28.84 F ATOM 5887 N PRO F 3 80.463 37.699 32.551 1.00 28.02 F ATOM 5888 CO GLIN F 2 79.690 36.081 30.462 1.00 27.76 F ATOM 5889 CA PRO F 3 80.363 37.575 28.660 1.00 28.68 F ATOM 5890 CB PRO F 3 80.363 37.575 28.660 1.00 28.68 F ATOM 5891 CG PRO F 3 80.370 36.332 28.198 1.00 27.76 F ATOM 5892 C PRO F 3 80.370 36.332 28.198 1.00 27.76 F ATOM 5893 C PRO F 3 80.370 36.332 28.198 1.00 27.76 F ATOM 5894 N PHE F 4 79.212 30.559 27.466 1.00 27.24 F ATOM 5895 CB PRO F 3 80.370 36.332 28.198 1.00 27.76 F ATOM 5896 CD PRO F 5 80.409 32.738 26.943 1.00 27.24 F ATOM 5897 CG PRE F 4 79.524 27.989 28.565 1.00 34.18 F ATOM 5896 CD PRO F 5 83.391 31.892 27.552 1.00 28.01 F ATOM 5896 CD PRO F 5 83.391 31.892 27.466 1.00 22.79 F ATOM 5897 CG PRE F 4 79.524 27.989 28.565 1.00 31.18 F ATOM 5890 CG PRO F 5 83.391 31.892 27.00 21.00 21.18 F	MOTA	5866	CD	ARG	E	189	83.030	83.499	11.045	1.00 63.51	B
ATOM 5869 NH1 ARG E 189 85.578 84.766 11.183 1.00 69.41 E ATOM 5870 C ARG E 189 83.950 83.322 7.313 1.00 55.74 E ATOM 5873 N ALA E 190 83.950 83.182 7.666 1.00 56.16 E ATOM 5874 CA ALA E 190 84.950 84.734 3.964 1.00 59.97 E ATOM 5876 CA ALA E 190 84.650 84.734 3.964 1.00 59.97 E ATOM 5876 CA ALA E 190 84.654 86.378 6.971 1.00 62.25 E ATOM 5879 C LEU F 1 78.718 38.671 33.365 1.00 32.03 F ATOM 5880 O LEU F 1 </td <td>MOTA</td> <td>5867</td> <td>NE</td> <td>ARG</td> <td>E</td> <td>189</td> <td>83.580</td> <td>84.180</td> <td>12.218</td> <td>1.00 66.73</td> <td>E</td>	MOTA	5867	NE	ARG	E	189	83.580	84.180	12.218	1.00 66.73	E
ATOM 5870 NH2 ARG E 189 85.178 85.378 13.363 1.00 70.13 E ATOM 5871 C ARG E 189 83.950 83.952 7.866 1.00 55.74 E ATOM 5872 O ARG E 189 83.950 83.952 7.866 1.00 55.74 E ATOM 5873 N ALA E 190 84.920 84.557 5.435 1.00 58.53 E ATOM 5875 CB ALA E 190 84.920 84.557 5.435 1.00 60.08 E ATOM 5875 CB ALA E 190 84.950 84.734 3.964 1.00 59.97 E ATOM 5876 C ALA E 190 84.654 86.378 6.971 1.00 61.01 E ATOM 5877 O ALA E 190 84.654 86.378 6.971 1.00 62.25 E ATOM 5878 CW ALA E 190 86.338 86.479 5.558 1.00 61.01 E ATOM 5879 C LEU F 1 78.718 38.094 33.366 1.00 32.03 F ATOM 5880 C LEU F 1 79.818 38.571 33.658 1.00 32.07 F ATOM 5880 C LEU F 1 79.818 38.571 33.658 1.00 32.07 F ATOM 5881 N LEU F 1 76.219 38.100 33.307 1.00 33.21 F ATOM 5888 CA LEU F 1 77.432 38.678 33.953 1.00 32.59 F ATOM 5886 C GLN F 2 79.574 36.436 31.936 1.00 22.73 F ATOM 5886 C GLN F 2 79.609 36.081 30.067 1.00 62.25 F ATOM 5886 C GLN F 2 79.609 36.081 30.067 1.00 27.03 F ATOM 5888 C GLN F 2 78.578 37.069 32.531 1.00 32.03 F ATOM 5886 C GLN F 2 78.674 35.466 31.936 1.00 28.84 F ATOM 5888 CD FRO F 3 80.463 36.663 29.619 1.00 28.02 F ATOM 5888 CD FRO F 3 80.463 36.663 29.619 1.00 28.02 F ATOM 5889 CA FRO F 3 80.463 36.663 29.619 1.00 28.02 F ATOM 5889 CA FRO F 3 80.463 36.663 29.619 1.00 28.02 F ATOM 5889 CA FRO F 3 80.463 36.663 29.619 1.00 28.02 F ATOM 5889 CA FRO F 3 80.370 36.332 28.938 1.00 27.76 F ATOM 5899 CB FRO F 3 80.370 36.332 28.938 1.00 27.76 F ATOM 5891 CG FRO F 3 80.367 32.338 26.943 1.00 27.76 F ATOM 5891 CG FRO F 3 80.360 30.067 1.00 27.68 F ATOM 5892 C FRO F 3 80.370 36.332 28.938 1.00 27.76 F ATOM 5893 C PRO F 3 80.370 36.332 28.938 1.00 27.76 F ATOM 5893 C PRO F 3 80.370 36.332 28.939 1.00 22.18 F ATOM 5897 C PRO F 3 80.360 30.300 1.00 27.18 F ATOM 5897 C PRO F 3 80.360 30.300 30.0000 30.0000 30.0000 30.0000 30.0000 30.0000 30.0000 30.0000 30.0000 30.0000 30.0000 30.	MOTA	5868	\mathbf{cz}	ARG	E	189	84.771	84.771	12.255	1.00 68.44	B
ATOM 5871 C ARG B 189 83.950 83.322 7.313 1.00 55.74 E ATOM 5872 O ARG B 189 85.043 83.162 7.866 1.00 56.16 E ATOM 5873 N ALA B 190 83.796 83.962 6.156 1.00 56.16 E ATOM 5873 N ALA B 190 84.920 84.557 5.435 1.00 60.08 E ATOM 5875 CB ALA B 190 84.550 84.734 3.964 1.00 59.97 E ATOM 5876 C ALA B 190 84.550 84.734 3.964 1.00 59.97 E ATOM 5876 C ALA B 190 84.654 86.378 6.971 1.00 62.25 E ATOM 5878 OXT ALA B 190 84.654 86.378 6.971 1.00 62.25 E ATOM 5878 OXT ALA B 190 84.654 86.378 6.971 1.00 62.25 E ATOM 5878 OXT ALA B 190 84.654 86.378 6.971 1.00 62.25 E ATOM 5878 OXT ALA B 190 84.654 86.378 33.658 1.00 30.77 F ATOM 5880 O LEU F 1 79.818 38.594 33.658 1.00 30.77 F ATOM 5881 N LEU F 1 76.219 38.100 33.307 1.00 33.21 F ATOM 5883 N GLNF 2 78.578 37.069 32.531 1.00 30.37 F ATOM 5883 N GLNF 2 79.744 36.436 31.936 1.00 22.59 F ATOM 5885 C GLN F 2 79.609 36.081 30.462 1.00 22.93 F ATOM 5885 C GLN F 2 79.609 36.081 30.462 1.00 22.93 F ATOM 5886 O GLN F 2 79.609 36.081 30.462 1.00 22.93 F ATOM 5886 C GLN F 2 79.609 36.081 30.462 1.00 22.93 F ATOM 5886 C GLN F 2 79.609 36.081 30.462 1.00 22.93 F ATOM 5886 C GLN F 3 80.463 36.663 29.619 1.00 28.84 F ATOM 5887 N PRO F 3 80.463 36.663 29.619 1.00 28.84 F ATOM 5888 CD PRO F 3 80.463 36.663 29.619 1.00 28.02 F ATOM 5889 CA PRO F 3 80.463 37.298 27.552 1.00 28.01 F ATOM 5890 CB PRO F 3 80.370 36.332 28.198 1.00 27.76 F ATOM 5891 CG PRO F 3 80.370 36.332 28.198 1.00 27.76 F ATOM 5893 O PRO F 3 80.370 36.332 28.198 1.00 27.76 F ATOM 5895 CA PHE F 4 79.243 31.905 26.849 1.00 27.24 F ATOM 5895 CA PHE F 4 79.435 30.384 28.823 1.00 33.24 F ATOM 5896 CD PHE F 4 79.435 30.384 28.823 1.00 33.24 F ATOM 5895 CA PHE F 4 79.435 30.384 28.823 1.00 33.24 F ATOM 5895 CA PHE F 4 79.564 22.939 24.586 1.00 24.75 F ATOM 5900 CEJ PHE F 4 79.564 22.939 24.586 1.00 22.18 F ATOM 5901 CC PHE F 4 79.564 22.939 24.586 1.00 22.18 F ATOM 5903 C PHE F 4 79.564 22.939 24.586 1.00 22.18 F ATOM 5900 CC PHE F 5 81.319 31.820 24.618 1.00 22.93 F ATOM 5900 CC PHE F 5 81.329 31.340 24.565 27.10 1.00 22.93 F ATOM 5900	MOTA	5869	NH1	ARG	B	189	85.553	84.766	11.183	1.00 69.41	
ATOM 5872 O ARG B 189 85.043 83.162 7.866 1.00 56.16 B ATOM 5873 N ALA B 190 84.920 84.557 5.435 1.00 60.08 E ATOM 5874 CA ALA E 190 84.920 84.557 5.435 1.00 60.08 E ATOM 5875 CE ALA E 190 84.950 84.734 3.964 1.00 59.97 B ATOM 5876 C ALA E 190 85.335 85.905 6.036 1.00 61.01 B ATOM 5877 O ALA E 190 84.654 86.378 6.971 1.00 62.25 E ATOM 5878 OXT ALA E 190 86.338 86.479 5.558 1.00 61.01 B ATOM 5878 OXT ALA E 190 86.338 86.479 5.558 1.00 30.77 F ATOM 5880 O LEU F 1 79.818 38.094 33.366 1.00 30.77 F ATOM 5881 N LEU F 1 76.219 38.100 33.307 1.00 33.21 F ATOM 5881 N LEU F 1 77.432 38.678 33.953 1.00 32.59 F ATOM 5883 N GLN F 2 78.578 37.069 32.531 1.00 30.39 F ATOM 5884 CA GLN F 2 79.744 36.436 31.936 1.00 28.84 F ATOM 5885 C GLN F 2 79.744 36.436 31.936 1.00 28.84 F ATOM 5886 O GLN F 2 79.744 36.436 31.936 1.00 27.93 F ATOM 5886 CD GLN F 2 79.744 36.436 31.936 1.00 28.84 F ATOM 5887 N PRO F 3 80.463 36.663 29.619 1.00 27.93 F ATOM 5889 CA PRO F 3 80.463 36.663 29.619 1.00 28.02 F ATOM 5889 CA PRO F 3 80.463 36.663 29.619 1.00 28.60 F ATOM 5889 CB PRO F 3 80.463 37.288 CD PRO F 3 80.463 37.288 CD 8.68 F ATOM 5890 CB PRO F 3 80.463 37.288 CD 8.68 F ATOM 5891 CG PRO F 3 80.463 37.288 CD 8.68 F ATOM 5893 C PRO F 3 80.4774 34.872 28.030 1.00 27.76 F ATOM 5893 O PRO F 3 80.370 37.282 28.596 1.00 28.68 F ATOM 5895 CB PRO F 3 80.4774 34.872 28.030 1.00 27.76 F ATOM 5895 CB PRO F 3 80.4774 34.872 28.030 1.00 27.76 F ATOM 5895 CB PRO F 3 80.4774 34.872 28.030 1.00 27.78 F ATOM 5895 CB PRO F 3 80.4774 34.872 28.030 1.00 27.78 F ATOM 5895 CB PRO F 3 80.774 34.872 28.030 1.00 27.24 F ATOM 5895 CB PRO F 3 80.774 34.872 28.030 1.00 27.24 F ATOM 5895 CB PRO F 3 80.774 34.872 28.030 1.00 27.24 F ATOM 5895 CB PRO F 3 80.774 34.872 28.030 1.00 27.24 F ATOM 5895 CB PRO F 3 80.774 34.872 28.030 1.00 27.18 F ATOM 5895 CB PRO F 5 80.487 57.572 29.856 1.00 28.41 F ATOM 5895 CB PRO F 5 80.487 57.572 29.856 1.00 28.41 F ATOM 5895 CB PRO F 5 80.487 57.572 29.856 1.00 28.41 F ATOM 5890 CB PRO F 5 80.487 57.572 29.856 1.00 28.41 F ATOM 5890 CB P	MOTA	5870	NH2								
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ATOM 5905 N PRO F 5 82.460 32.065 25.771 1.00 22.79 F ATOM 5906 CD PRO F 5 83.191 31.820 27.029 1.00 21.18 F ATOM 5907 CA PRO F 5 83.349 31.882 24.618 1.00 21.18 F ATOM 5908 CB PRO F 5 84.715 32.140 25.218 1.00 20.19 F ATOM 5909 CG PRO F 5 84.587 31.450 26.544 1.00 20.99 F ATOM 5910 C PRO F 5 83.291 30.524 23.949 1.00 20.28 F ATOM 5911 O PRO F 5 82.796 29.559 24.521 1.00 19.48 F ATOM 5912 N GLN F 6 83.818 30.456 22.730 1.00 21.24 F ATOM 5913 CA GLN F 6 83.848 29.200 21.983 1.00 19.98 F ATOM 5914 CB GLN F 6 83.665 29.450 20.484 1.00 18.71 F	ATOM	5903	С	PHE	F	4	81.227	32.588			
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MOTA	5916	CD	GFN		6	82.255	30.247	18.537	1.00 22.29	F
ATOM	5917	OE1	GLN	F	6	82.612	29.368	17.740	1.00 21.53	F
ATOM	5918	NB2	GLN	F	6	81.802	31.429	18.138	1.00 20.02	F
ATOM	5919	С	GLN	F	6	85.213	28.548	22.213	1.00 20.47	F
ATOM	5920	ō	GLN		6	86.243	29.204	22.099	1.00 18.48	F
ATOM	5921	N	PRO		7	85.229	27.256	22.575	1.00 21.16	F
MOTA	5922	CD	PRO	F	7	84.071	26.494	23.084	1.00 20.59	F
ATOM	5923	CA	PRO	P	7	86.471	26.520	22.813	1.00 21.61	F
ATOM	5924	CB	PRO		7	86.037	25.444	23.797	1.00 23.40	F
MOTA	5925	CG	PRO		7	84.649	25.123	23.311	1.00 19.67	F
ATOM	5926	C	PRO	F	7	86.996	25.897	21.521	1.00 23.00	F
ATOM	5927	0	PRO	F	7	86.219	25.601	20.610	1.00 23.19	F
MOTA	5928	N	GLU		8	88.312	25.714	21.438	1.00 21.78	F
					8				1.00 23.12	F
ATOM	5929	CA	GTA			88.904	25.068	20.279		
ATOM	5930	CB	GŢŪ	F	8	90.297	25.632	19.968	1.00 24.50	F
MOTA	5931	CG	GLU	F	8	91.086	24.834	18.915	1.00 26.16	F
ATOM	5932	CD	GΤΩ	F	8	90.360	24.697	17.576	1.00 31.57	F
	5933		GTA		8	89.250	24.114	17.540	1.00 33.65	F
ATOM										
MOTA	5934	OE2	GTA	F	8	90.903	25.171	16.555	1.00 30.66	F
ATOM	5935	C	GLU	F	8	89.005	23.608	20.680	1.00 22.95	F
ATOM	5936	0	GLU	F	8	89.289	23.292	21.833	1.00 23.25	F
ATOM	5937	N	LEU		9	88.756	22.712	19.741	1.00 24.74	F
ATOM	5938	CA	LEU		9	88.815	21.292	20.047	1.00 27.30	F
MOTA	5939	CB	PEA	F	9	87.729	20.549	19.272	1.00 25.73	F
ATOM	5940	CG	LEU	F	9	86.302	21.051	19.494	1.00 29.20	F
ATOM	5941		LEU		9	85.338	20.235	18.645	1.00 28.18	P
MOTA	5942		LEU		9	85.938	20.943	20.967	1.00 29.61	P
ATOM	5943	С	LEU	F	9	90.178	20.707	19.712	1.00 28.17	F
ATOM	5944	0	LEU	F	9	90.715	20.940	18.631	1.00 26.94	F
ATOM	5945	N	PRO		10	90.765	19.947	20.647	1.00 30.38	F
										F
ATOM	5946	CD	PRO		10	90.365	19.707	22.044	1.00 30.47	
MOTA	5947	CA	PRO	F	10	92.076	19.355	20.370	1.00 34.24	F
MOTA	5948	CB	PRO	F	10	92.556	18.915	21.752	1.00 32.97	F
MOTA	5949	CG	PRO	F'	10	91.282	18.561	22.448	1.00 31.98	F
ATOM	5950	c	PRO		10	91.985	18.188	19.393	1.00 35.94	F
MOTA	5951	0	PRO		10	90.993	17.461	19.376	1.00 38.70	F
ATOM	5952	N	TYR	P	11	93.016	18.031	18.570	1.00 37.40	F
MOTA	5953	CA	TYR	F	11	93.075	16.936	17.609	1.00 38.84	F
ATOM	5954	CB	TYR		11	92.126	17.176	16.434	1.00 38.73	F
									1.00 39.56	F
ATOM	5955	CG	TYR		11	92.017	15.969	15.539		
MOTA	5956	CD1	TYR	F	11	91.294	14.848	15.942	1.00 39.88	F
ATOM	5957	CE1	TYR	F	11	91.254	13.697	15.164	1.00 39.49	F
ATOM	5958	CD2	TYR	F	11	92.698	15.913	14.327	1.00 39.73	F
MOTA	5959		TYR		11	92.668	14.765	13.537	1.00 40.44	F
										P
ATOM	5960	CZ	TYR		11	91.945	13.659	13.964	1.00 40.29	
MOTA	5961	OH	TYR	F	11	91.921	12.514	13.200	1.00 40.03	F
ATOM	5962	С	TYR	F	11	94.498	16.781	17.077	1.00 40.23	F
ATOM	5963	0	TYR	F	11	95.102	15.708	17.300	1.00 41.88	P
	5964	OXT			11	94.988	17.742	16.443	1.00 40,58	F
MOTA										
MOTA	5965	0	HOH		1	37.560	11.197	17.272	1.00 17.47	H
MOTA	5966	0	HOH	H	2	81.295	26.543	20.573	1.00 15.95	H
ATOM	5967	0	HOH	H	3	43.884	23.627	16.726	1.00 14.83	H
MOTA	5968	0	HOH	н	4	89.230	61.015	16.512	1.00 19.10	H
ATOM	5969	ō	HOH		5	92.090	40.877	18.768	1.00 15.59	н
ATOM	5970	0	HOH		6	57.686	14.054	4.407	1.00 20.02	Н
ATOM	5971	0	HOH	H	7	87.607	31.423	22.217	1.00 11.29	H
MOTA	5972	0	HOH	H	8	31.815	41.479	5.673	1.00 23.91	H
ATOM	5973	0	нон		9	46.112	3.594	18.714	1.00 20.15	H
								15.551	1.00 22.39	H
ATOM	5974	0	HOH		10	86.724	67.786			
MOTA	5975	0	HOH	H	11	42.599	14.833	17.213	1.00 16.12	H
ATOM	5976	0	HOH	H	12	93.679	37.081	11.737	1.00 15.03	H
MOTA	5977	0	нон	н	13	50.288	0.581	25.262	1.00 13.69	H
MOTA	5978	Ö	нон		14	96.256	37.853	25.291	1.00 12.90	н
MOTA	5979	0	нон		15	90.711	30.936	37.307	1.00 31.88	H
ATOM	5980	0	HOH	H	16	80.045	39.846	25.144	1.00 33.11	Ħ
MOTA	5981	0	HOH	H	17	80.708	45.662	11.514	1.00 41.56	H
ATOM	5982	ō	нон		18	42.215	0.119	11.193	1.00 15.83	H
			нон			95.828		5.930	1.00 27.67	H
MOTA	5983	0			19		50.485			
MOTA	5984	0	HOH		20	48.809	37.278	14.928	1.00 36.10	н,
MOTA	5985	0	HOH	Η	21	47.553	-0.403	11.823	1.00 14.62	H
								10 100	7 00 00 00	H
		0	HOH	H	22	94.554	76.132	19.122	1.00 83.80	п
MOTA	5986	0	HOH			94.554	76.132 48.460			
MOTA MOTA	5986 5987	0	HOH	Н	23	83.295	48.460	17.328	1.00 17.64	H
MOTA	5986			H						

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ATOM	5990	0	нон н	26	47.640	0.006	20.312	1.00 18.95	H
MOTA	5991	0	нон н	27	46.987	29.359	11.916	1.00 21.84	H
MOTA	5992	0	нон н	28	88.283	37.229	11.279	1.00 21.34	H
MOTA	5993	0	HOH H	29	49.878	-9.043	36.424	1.00 32.47	H
MOTA	5994	0	HOH H	30	82.777	39.366	24.935	1.00 24.79	H,
MOTA	5995	0	нон н	31	72.919	25.704	15.123	1.00 18.09	H
ATOM	5996	o	нон н	32	86.830	25.153	13.558	1.00 24.14	H
ATOM	5997	ŏ	нон н	33	43.152	5.651	13.774	1.00 19.96	н
MOTA	5998	0	нон н	34	100.654	27.732	5.367	1.00 34.73	H
MOTA	5999	0	HOH H	35	48.550	32.122	26.894	1.00 20.17	H
ATOM	6000	0	HOH H	36	78.728	36.578	6.822	1.00 32.92	H
MOTA	6001	0	нон н	37	89.361	11.980	24.953	1.00 51.75	H
MOTA	6002	0	нон н	38	90.411	24.657	31.926	1.00 28.29	H
ATOM	6003	0	нон н	39	80.690	24.233	8.462	1.00 22.43	H
MOTA	6004	ō	нон н	40	83.769	65.973	-5.489	1.00 21.06	H
MOTA	6005	ō	нон н	41	87.710	34.692	7.008	1.00 22.47	н
ATOM	6006	0	нон н	42	38.997	4.521	15.299	1.00 25.36	H
MOTA	6007	0	нон н	43	94.223	46.644	24.674	1.00 32.67	H
MOTA	6008	0	нон н	44	35.150	15.757	26.294	1.00 29.03	H
ATOM	6009	0	нон н	45	85.059	24.652	18.280	1.00 25.63	H
MOTA	6010	0	нон н	46	67.739	6.320	18.991	1.00 43.67	H
MOTA	6011	0	нон н	47	92.376	63.977	12.866	1.00 32.46	H
MOTA	6012	o	нон н	48	91.526	49.479	22.504	1.00 29.70	н
ATOM	6013	ō	нон н	49	56.333	-2.088	24.733	1.00 28.53	H
MOTA	6014	0	нон н	50	100.482	53.937	3.942	1.00 52.26	H
MOTA	6015	0	нон н	51	48.244	18.753	22.918	1.00 44.88	H
MOTA	6016	0	нон н	52	32.577	-0.558	6.769	1.00 33.70	H
ATOM	6017	0	нон н	53	47.162	26.527	12.972	1.00 29.72	H
MOTA	6018	0	нон н	54	98.621	66.834	5.100	1.00 52.20	H
ATOM	6019	ō	нон н	55	88.106	52.134	17.293	1.00 21.13	H
ATOM	6020	ŏ	нон н	56	59.655	31.307	17.069	1.00 25.89	H
					73.562			1.00 23.51	
ATOM	6021	0	нон н	57		24.323	12.997		H
MOTA	6022	0	нон н	58	43.748	32.725	20.165	1.00 52.72	H
ATOM	6023	0	нон н	59	26.392	-7.072	11.400	1.00 26.20	H
ATOM	6024	0	нон н	60	83.955	73.751	16.805	1.00 18.19	H
MOTA	6025	0	нон н	61	46.229	-19.766	10.675	1.00 28.79	H
MOTA	6026	0	нон н	62	52.436	38.720	16.630	1.00 28.35	H
ATOM	6027	0	нон н	63	60.555	9.392	19.914	1.00 28.43	н
ATOM	6028	ō	нон н	64	62.105	2.197	11.948	1.00 33.33	н
ATOM	6029	ō	нон н	65		-12.059	13.631	1.00 21.32	н
MOTA	6030	0	нон н	66	65.876	23.972	14.155	1.00 21.11	н
MOTA	6031	0	нон н	67	84.702	18.013	5.666	1.00 19.12	H
ATOM	6032	0	нон н	68	64.715	11.655	15.936	1.00 28.72	H
MOTA	6033	0	нон н	69	85.418	74.949	14.820	1.00 27.90	H
ATOM	6034	0	нон н	70	77.974	25.419	23.038	1.00 42.15	H
ATOM	6035	0	нон н	71	65.805	8.484	20.741	1.00 44.01	H
MOTA	6036	0	нон н	72	51,276	26.045	10.800	1.00 28.36	н
ATOM	6037	ō	нон н	73	65.226	22.195	25.831	1.00 36.11	н
	6038	ŏ	нон н	74	101.567	46.068	1.107	1.00 53.81	н
ATOM									
ATOM	6039	0	нон н	75	32.615	31.234	1.517	1.00 21.03	H
MOTA	6040	0	HOH H	76	42.100	-0.001	13.802	1.00 23.44	H
MOTA	6041	0	нон н	77	35.124	40.614	14.668	1.00 27.61	H
MOTA	6042	0	нон н	78	92.548	46.813	7.595	1.00 31.64	н
ATOM	6043	0	нон н	79	34.670	13.941	14.778	1.00 22.87	н
ATOM	6044	0	нон н	80	98.527	27.671	28.270	1.00 42.07	H
ATOM	6045	0	нон н	81	30.588	36.032	16.540	1.00 37.52	н
ATOM	6046	o	нон н	82	89.345	42.957	13.940	1.00 22.73	H
ATOM	6047	ō	нон н	83	92.891	18.085	10.698	1.00 32.35	H
MOTA	6048	0	нон н	84	90.050	48.556	16.519	1.00 27.30	Н
MOTA	6049	0	нон н	85	110.812	49,549	15.813	1.00 27.68	H
MOTA	6050	0	нон н	86	75.872	21.668	2.499	1.00 39.37	H
MOTA	6051	0	нон н	87	52.567	14.010	7.270	1.00 34.20	H
MOTA	6052	0	нон н	88	69.016	32.569	12.651	1.00 36.96	H
ATOM	6053	0	нон н	89	96.637	25.945	31.742	1.00 37.26	H
ATOM	6054	ŏ	нон н	90		-12.998	8.560	1.00 22.82	H
MOTA	6055	ō	нон н	91	113.021	48.469	17.945	1.00 47.59	H
	6056	ŏ			34.266		23.930	1.00 31.02	H
ATOM			нон н	92		25.052			
MOTA	6057	0	нон н	93	51.464	31.946	19.300	1.00 15.75	H
MOTA	6058	0	нон н	94	80.054	50.912	15.041	1.00 25.94	H
ATOM	6059	0	нон н	95		-13.432	16.393	1.00 39.73	H
MOTA	6060	0	нон н	96	57.701		7.708	1.00 25.27	H
MOTA	6061	0	нон н	97	80.838	52.853	26.436	1.00 27.67	H
ATOM	6062	0	нон н	98	58.205	13.023	20.294	1.00 27.57	H
MOTA	6063	0	нон н	99	41.832		15.601	1.00 27.32	н
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MOTA	6064	0	HOH H 100	72.807	29.880	11.618	1.00 28.05	H
MOTA	6065	0	HOH H 101	48.499	5.079	4.053	1.00 38.72	H
MOTA	6066	0	нон н 102	100.679	66.408	9.019	1.00 36.21	H
ATOM	6067	0	HOH H 103	45.023	41.442	11.747	1.00 42.72	H
ATOM	6068	ŏ	HOH H 104					
				83.296	63.483	-2.738	1.00 27.46	H
MOTA	6069	0	нон н 105	85.067	29.522	34.732	1.00 35.62	H
ATOM	6070	0	HOH H 106	72.272	53.390	15.314	1.00 38.75	H
MOTA	6071	0	HOH H 107	80.600	27.688	5.225	1.00 26.04	н
ATOM	6072	0	HOH H 108	71.251		16.503	1.00 29.08	H
ATOM	6073		нон н 109					
		0		88.274		19.510	1.00 26.70	H
MOTA	6074	0	HOH H 110	43.031	4.836	7.813	1.00 38.59	H
MOTA	6075	0	HOH H 111	101.304	35.384	4.755	1.00 43.53	Н
MOTA	6076	0	HOH H 112	44.554	10.725	19.619	1.00 21.38	H
MOTA	6077	0	HOH H 113	115.506	34.478	5.615	1.00 46.62	н
MOTA	6078	ō	HOH H 114		-25.634	9.802	1.00 42.69	H
MOTA	6079	0	HOH H 115		-33.304	20.170	1.00 61.12	H
MOTA	6080	0	HOH H 116	38.663	26.161	-2.715	1.00 31.39	H
ATOM	6081	0	HOH H 117	105.197	41.384	18.739	1.00 38.53	H
MOTA	6082	0	HOH H 118	38.437	-12.372	18.422	1.00 32.47	н
ATOM	6083	0	HOH H 119	45.430	15.732	9.556	1.00 32.39	н
ATOM	6084	ŏ	HOH H 120	70.475	9.817			
						-1.029	1.00 53.38	H
MOTA	6085	0	HOH H 121	87.895	64.540	22.445	1.00 47.01	H
MOTA	6086	0	HOH H 122	39.337	36.650	16.644	1.00 25.21	H
ATOM	6087	0	HOH H 123	104.091	50.783	20.204	1.00 31.31	H
MOTA	6088	0	HOH H 124	72.528	13.825	20.909	1.00 62.81	H
MOTA	6089	ō	HOH H 125	55.353	-5.411	5.747	1.00 25.46	н
MOTA		ō						
	6090		HOH H 126	97.848	63.704	25.177	1.00 27.84	H
MOTA	6091	0	HOH H 127	89.799	75.117	14.074	1.00 49.56	Н
MOTA	6092	0	HOH H 128	96.226	35.565	0.211	1.00 40.25	H
ATOM	6093	0	HOH H 129	25.125	-15.445	19.161	1.00 37.04	H
ATOM	6094	0	нон н 130	90.627	52.974	9.649	1.00 22.70	н
ATOM	6095	ō	нон н 131	114.398	29.773			
						11.425	1.00 42.36	H
MOTA	6096	0	нон н 132	69.810	89.608	-0.164	1.00 53.48	H
MOTA	6097	0	HOH H 133	99.069	30.421	4.728	1.00 31.21	H
ATOM	6098	0	HOH H 134	37.335	49.129	5.746	1.00 43.90	H
MOTA	6099	0	нон н 135	77.753	73.821	17.600	1.00 50.43	H
MOTA	6100	0	нон н 136	44.853	33.208	11.090	1.00 21.26	н
MOTA	6101	ō	HOH H 137	88.697				
					80.608	-4.574	1.00 49.42	H
MOTA	6102	0	HOH H 138	62.018	-6.136	9.010	1.00 30.19	H
MOTA	6103	0	HOH H 139	35.964	-5.810	5.494	1.00 45.47	H
MOTA	6104	0	HOH H 140	73.968	65.480	8.013	1.00 43.93	H
MOTA	6105	0	HOH H 141	78.361	66.868	24.455	1.00 57.76	H
MOTA	6106	0	HOH H 142	53.527	3.199	22.332	1.00 32.95	н
ATOM	6107	ō	HOH H 143		-6.530			
				56.018		25.205	1.00 42.75	H
MOTA	6108	0	HOH H 144	82.930	52.617	28.345	1.00 32.35	H
MOTA	6109	0	HOH H 145	28.607	-21.313	24.210	1.00 48.87	H
MOTA	6110	0	HOH H 146	86.079	41.197	35.698	1.00 36.97	H
ATOM	6111	0	HOH H 147	35.017	8.399	11.516	1.00 32.21	H
ATOM	6112	0	HOH H 148		-19.905	17.166	1.00 41.53	н
MOTA	6113	ō	HOH H 149	55.504	20.659	6.959	1.00 36.63	н
			HOH H 150					
MOTA	6114	0		106.046	47.260	19.571	1.00 30.60	H
ATOM	6115	0	HOH H 151	108.769	26.147	5.447	1.00 48.82	H
MOTA	6116	0	HOH H 152	38.689	17.576	4.331	1.00 39.07	H
MOTA	6117	0	HOH H 153	97.787	62.580	8.740	1.00 29.61	H
ATOM	6118	0	HOH H 154	59.501	-12.817	20.769	1.00 50.36	H
ATOM	6119	ō	нон н 155	47.887	40.072	-4.641	1.00 51.05	H
MOTA	6120	0	нон н 156	60.057		27.477	1.00 40.66	H
ATOM	6121	0	нон н 157	67.048	27.841	20.873	1.00 39.66	н
ATOM	6122	0	HOH H 158	37.028	32.932	18.669	1.00 37.23	H
ATOM	6123	0	HOH H 159	121.780	18.693	-3.076	1.00 46.64	H
ATOM	6124	0	HOH H 160	39.196		27.271	1.00 29.99	H
ATOM	6125	ŏ	HOH H 161	113.285		19.561	1.00 39.04	H
ATOM	6126		HOH H 162					
		0		43.379		19.370	1.00 27.58	H
MOTA	6127	0	HOH H 163	91.636		11.885	1.00 54.73	H
MOTA	6128	0	HOH H 164	113.381	46.844	20.020	1.00 54.22	H
MOTA	6129	0	HOH H 165	79.238	62.082	24.112	1.00 36.07	H
MOTA	6130	0	нон н 166	27.985	32.355	18.424	1.00 36.25	H
ATOM	6131	ō	HOH H 167		-10.661	20.615	1.00 9.89	H
ATOM	6132	ŏ	HOH H 168	93.577		20.182	1.00 14.03	H
MOTA	6133	0	нон н 169	97.912		7.309	1.00 24.22	H
MOTA	6134	0	HOH H 170	69.616	4.375	18.521	1.00 38.01	H
MOTA	6135	0	HOH H 171	80.870	25.194	6.002	1.00 21.84	H
ATOM	6136	0	HOH H 172	50.564	12.887	5.906	1.00 32.25	H
ATOM	6137	ò	HOH H 173	88.207		13.919	1.00 19.68	н
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ATOM	6138	0	HOH H 174	93.800	47.651	27.174	1.00 41.65	H
ATOM	6139	0	HOH H 175	52.842	0.304	25.210	1.00 28.07	H
ATOM	6140	0	нон н 176	66.457	4.742	14.051	1.00 28.64	H
ATOM	6141	0	HOH H 177	36.948	12.416	15.109	1.00 28.66	H
MOTA	6142	0	HOH H 178	103.292	41.793	7.607	1.00 28.51	H
MOTA	6143	0	HOH H 179	86.476	36.035	9.339	1.00 27.43	Ħ
MOTA	6144	0	HOH H 180	82.262	41.159	26.845	1.00 24.13	H
ATOM	6145	0	HOH H 181	32.348	15.030	26.400	1.00 30.06	H
ATOM	6146	0	HOH H 182	69.916	30.709	14.482	1.00 42.81	н
ATOM	6147	0	HOH H 183	48.060	10.142	26.751	1.00 49.12	H
ATOM	6148	0	HOH H 184	45.863	-9.131	37.252	1.00 43.70	Ħ
ATOM	6149	0	HOH H 185	32.095	-3.806	34.251	1.00 41.46	H
MOTA	6150	0	HOH H 186	108.258	31.975	8.914	1.00 33.62	H
ATOM	6151	0	HOH H 187	99.465	64.293	8.210	1.00 54.43	H
ATOM	6152	0	HOH H 188	74.677	30.785	27.841	1.00 28.20	H
MOTA								
	6153	0	нон н 189	44.953	0.968	35.892	1.00 32.25	H
MOTA	6154	0	HOH H 190	88.523	27.792	36.268	1.00 30.83	H
ATOM	6155	0	HOH H 191	37.736	8.611	11.729	1.00 38.92	н
MOTA	6156	o	HOH H 192	35.988	45.178	12.964	1.00 33.85	H
MOTA	6157	0	HOH H 193	77.222	68.027	1.401	1.00 27.02	H
ATOM	6158	0	HOH H 194	63.326	-8.764	15.926	1.00 38.46	H
MOTA	6159	0	HOH H 195	109.635	61.489	27.644	1.00 52.79	н
MOTA	6160	0	нон н 196	101.299	67.528	11.319	1.00 38.92	H
ATOM	6161	0	нон н 197	77.295	56.116	25.768	1.00 36.83	H
ATOM	6162	0	HOH H 198	81.538	22.288	0.320	1.00 47.08	H
MOTA	6163	0	HOH H 199	55.989	3.900	0.756	1.00 46.35	H
MOTA	6164	0	HOH H 200	66.200	40.514	17.513	1.00 43.54	H
MOTA	6165	0	HOH H 201	40.497	-1.046	9.238	1.00 27.84	H
			HOH H 202	57.171		8.258	1.00 52.74	
ATOM	6166	0			27.504			H
MOTA	6167	0	HOH H 203	44.592	-6.430	37.531	1.00 37.55	H
MOTA	6168	0	HOH H 204	26.892	-1.642	9.494	1,00 55.58	н
ATOM	6169	0	HOH H 205	83.350	58.389	2.759	1.00 46.24	H
MOTA	6170	0	нон н 206	112.353	45.284	9.770	1.00 30.99	H
ATOM	6171	0	HOH H 207	86.315	23.927	16.100	1.00 41.36	H
MOTA	6172	0	HOH H 208	67.053	45.396	12.396	1.00 31.02	н
ATOM	6173	0	нон н 209	111.609	60.418	8.362	1.00 52.01	H
MOTA	6174	0	HOH H 210	91.254	47.553	32.752	1.00 41.71	H
MOTA	6175	0	HOH H 211	88.489	39.944	11.117	1.00 34.00	H
ATOM	6176	0	HOH H 212	104.972	69.233	16.415	1.00 37.26	H
		-						
ATOM	6177	0	HOH H 213	23.462	39.893	6.692	1.00 56.45	H
MOTA	6178	0	HOH H 214	84.114	54.447	-1.718	1.00 42.58	H
ATOM	6179	0	HOH H 215	105.045	66.068	22.775	1.00 24.48	н
ATOM	6180	0	HOH H 216	85.378	52.388	17.025	1.00 37.91	H
MOTA	6181	0	HOH H 217	91.411	30.837	4.259	1.00 23.59	H
ATOM	6182	0	HOH H 218	99.019	37.803	25.178	1.00 37.20	H
ATOM	6183	0	нон н 219	88.866	41.183	35.781	1.00 42.88	H
MOTA	6184	0	нон н 220	66.946	25.931	12.530	1.00 45.53	H
ATOM	6185	0	HOH H 221	83.809	61.544	-0.645	1.00 32.51	н
ATOM			HOH H 222	91.766	28.386	3.286	1.00 29.97	H
	6186	0						
MOTA	6187	0	HOH H 223	83.302	45.674	11.423	1.00 40.65	H
ATOM	6188	0	HOH H 224	59.198	3.628	18.904	1.00 22.61	H
ATOM	6189	0	HOH H 225	34.553	-11.852	5.930	1.00 29.77	H
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MOTA	6190	0	HOH H 226	88.953	22.712	24.560	1.00 23.54	H
ATOM	6191	0	HOH H 227	108.379	54.102	21.160	1.00 30.79	H
ATOM	6192	0	HOH H 228	44.957	16.820	6.827	1.00 37.14	H
ATOM	6193	ŏ	HOH H 229	105.872	50.217	22.393	1.00 33.77	H
MOTA	6194	0	нон н 230	40.390	52.287	-1.729	1.00 62.00	H
ATOM	6195	0	HOH H 231	103.837	27.586	24.806	1.00 50.76	H
ATOM	6196	0	HOH H 232	50.931	9.397	25.207	1.00 40.65	H
					2.382			н
MOTA	6197	0	HOH H 233	64.739		27.973	1.00 46.98	
MOTA	6198	0	HOH H 234	38.363	0.460	8.402	1.00 28.58	H
MOTA	6199	0	нон н 235	73.577	50.129	18.561	1.00 36.68	H
ATOM	6200	ŏ	нон н 236	100.912	58.519	6.876	1.00 36.99	н
MOTA	6201	0	нон н 237	100.664	26.841	26.380	1.00 36.27	H
ATOM	6202	0	HOH H 238	82.528	48.080	12.484	1.00 44.97	H
ATOM	6203	ō	нон н 239	70.870	44.782	13.746	1.00 26.53	H
ATOM	6204	0	HOH H 240	71.914	-9.049	17.302	1.00 59.29	H
MOTA	6205	0	HOH H 241	28.024	9.146	32.377	1.00 43.91	H
MOTA	6206	0	HOH H 242	55.531	-2.470	4.880	1.00 50.20	H
ATOM		ŏ		63.362		21.334	1.00 30.95	H
	6207		HOH H 243		16.623			
MOTA	6208	0	HOH H 244	71.813	27.548	12.914	1.00 54.77	H
MOTA	6209	٥	HOH H 245	22.793	-3.930	12.731	1.00 39.10	H
ATOM	6210	0	HOH H 246	73.087	44.091	34.124	1.00 47.86	H
								н
MOTA	6211	0	HOH H 247	48.717	31.774	19.850	1.00 33.46	17

MOTA	6212	0	HOH H 248	100.851	61.218	7.741	1.00 35.49	H
MOTA	6213	0	HOH H 249	116.291	47.311	12.227	1.00 49.67	H
MOTA	6214	0	HOH H 250	99.469	40.748	22.418	1.00 25.82	H
MOTA	6215	0	HOH H 251	52.271	4.031	24.614	1.00 44.68	H
MOTA	6216	0	HOH H 252	106.629	40.298	32.271	1.00 59.44	H
		ŏ						
ATOM	6217		нон н 253	45.587	-9.303	3.049	1.00 26.81	H
ATOM	6218	0	HOH H 254	52.547	-9.432	27.670	1.00 45.08	H
MOTA	6219	0	нон н 255	75.854	21.157	27.640	1.00 42.33	H
MOTA	6220	0	нон н 256	82.119	63.444	23.430	1.00 37.84	H
MOTA	6221	0	HOH H 257	104.091	38.660	18.936	1.00 30.29	H
MOTA	6222	0	HOH H 258	79.477	56.121	8.190	1.00 39.16	H
MOTA	6223	0	нон н 259	101.351	32.257	5.631	1.00 29.94	H
MOTA	6224	0	HOH H 260	93.989	23.313	31.488	1.00 35.30	H
ATOM	6225	0	HOH H 261	28.754	-1.723	6.977	1.00 36.90	H
ATOM		ō	HOH H 262				1.00 49.06	
	6226			93.007	48.370	9.901		H
MOTA	6227	0	HOH H 263	82.990	88.137	9.529	1.00 39.70	H
ATOM	6228	0	HOH H 264	118.031	51.582	0.542	1.00 36.21	H
ATOM	6229	0	нон н 265	21.682	15.046	11.602	1.00 62.29	H
MOTA	6230	0	нон н 266	34.210	24.576	5.314	1.00 18.89	H
MOTA	6231	0	HOH H 267	85.829	40.095	14.911	1.00 25.26	H
ATOM	6232	0	HOH H 268	102.070	38.308	21.059	1.00 41.79	H
MOTA	6233	0	нон н 269	41.071	-2.346	7.039	1.00 38.87	H
MOTA	6234	0	HOH H 270	68.717	3.686	16.083	1.00 37.79	H
MOTA	6235	0	HOH H 271	27.094	-12.649	12.753	1.00 29.26	н
MOTA	6236	0	нон н 272	36.426	24.744	4.145	1.00 45.88	H
ATOM	6237	0	HOH H 273	88.670	31.858	5.525	1.00 39.43	H
ATOM	6238	0	HOH H 274	90.819	38.524	36.028	1.00 30.15	H
ATOM	6239	0	нон н 275	90.790	49.861	10.317	1.00 39.97	H
MOTA	6240	0	HOH H 276	77.026	11.969	13.970	1.00 44.87	H
ATOM	6241	0	HOH H 277	36.555	12.078	12.344	1.00 40.47	H
ATOM	6242	ō	HOH H 278		7.302	24.972	1.00 49.30	
				52.331				H
MOTA	6243	0	HOH H 279	92.612	33.229	3.564	1.00 40.55	H
ATOM	6244	0	HOH H 280	83.546	64.142	25.612	1.00 50.28	н
ATOM	6245	0	HOH H 281	28.206	-1.891	36.868	1.00 44.06	H
MOTA	6246	0	HOH H 282	93.185	20.914	30.917	1.00 44.51	H
ATOM	6247	0	HOH H 283	98.176	41.763	24.500	1.00 44.20	H
MOTA	6248	0	HOH H 284	29.174	-0.123	4.304	1.00 46.75	H
MOTA	6249	0	HOH H 285	79.206	77.643	14.919	1.00 30.21	H
ATOM	6250	0	HOH H 286	90.531	26.085	37.436	1.00 36.96	H
ATOM	6251	0	HOH H 287	55.726	0.396	21.054	1.00 49.55	H
MOTA	6252	ō	HOH H 288	111.246	30.915	19.699	1.00 42.91	н
MOTA	6253	0	HOH H 289	77.000	58.921	5.300	1.00 47.04	H
ATOM	6254	Ο,	HOH H 290	34.339	-9.458	5.288	1.00 25.50	H
MOTA	6255	0	HOH H 291	109.784	29.168	15.534	1.00 45.96	H
ATOM	6256	0	HOH H 292	93.674	48.853	29.650	1.00 48.76	H
ATOM	6257	0	нон н 293	92.299	47.066	3.801	1.00 37.41	H
MOTA	6258	0	HOH H 294	110.965	23.141	11.799	1.00 42.97	H
		ō		90.562				
ATOM	6259		HOH H 295		45.235	33.919	1.00 33.83	H
MOTA	6260	0	нон н 296	57,772	-10.500	25.018	1.00 49.78	H
MOTA	6261	0	HOH H 297	54.676	36.195	11.362	1.00 54.22	н
ATOM	6262	0	HOH H 298	107.263	59.234	5.282	1.00 56.05	H
MOTA	6263	0	нон н 299	70.560	48.918	1.476	1.00 49.72	H
MOTA.	6264	0	HOH H 300	84.037	38.916	5.971	1.00 39.33	H
MOTA	6265	0	HOH H 301	86.468	41.381	11.971	1.00 45.69	H
				24.400				
ATOM	6266	0	нон н 302		11.569	23.610	1.00 36.73	H
ATOM	6267	0	HOH H 303	73.087	79.808	7.028	1.00 46.20	H
ATOM	6268	0	HOH H 304	72.681	43.116	14.941	1.00 51.84	H
ATOM	6269		нон н 305	84.844	42.198	15.611	1.00 26.23	н
		0					-	
MOTA	6270	0	HOH H 306	54.135	19.007	24.978	1.00 27.41	H
ATOM	6271	0	нон н 307	67.044	10.459	18.465	1.00 44.92	н
MOTA	6272	0	нон н 308	82.262	49.436	14.864	1.00 39.04	. H
MOTA	6273	0	нон н 309	114.093	50.994	16.895	1.00 43.32	H
MOTA	6274	0	HOH H 310	64.428	3.092	30.590	1.00 43.29	H
MOTA	6275	0	HOH H 311	81.152	70.187	18.656	1.00 34.21	н
							1.00 55.00	
MOTA	6276	0	HOH H 312	74.596	81.584	-2.515		н
MOTA	6277	0	нон н 313	61.161	25.774	22.464	1.00 32.98	H
MOTA	6278	0	HOH H 314	53.149	-7.019	4.754	1.00 26.01	H
MOTA	6279	ō	нон н 315	44.571	8.317	33.567	1.00 40.32	н
MOTA	6280	0	нон н 316	82.293	49.769	10.587	1.00 35.22	H
ATOM	6281	0	HOH H 317	48.467	8.859	24.614	1.00 42.38	н
ATOM	6282	ō	HOH H 318	56.588	-8.027	4.728	1.00 44.65	н
MOTA	6283	0	нон н 319		-23.239	26.551	1.00 42.45	H
MOTA	6284	0	нон н 320	82.483	40.137	7.719	1.00 39.22	H
			нон н 321	82.063	19.937	23.440	1.00 35.69	н
ATOM	6285	0	DUD D 321					

ATOM 6286 a HOH H 322 106.025 63.366 22.616 1.00 31.93 Н MOTA 6287 ٥ HOH H 323 46.181 9.890 8.669 1.00 38.11 H ATOM 6288 HOH H 324 71.708 75.568 6.998 1.00 41.82 H ATOM 6289 0 HOH H 325 108.280 34.405 3.851 1.00 30.72 H ATOM 6290 0 HOH H 326 32.275 40.921 14.635 1.00 40.72 H ATOM 6291 0 нон н 327 37.556 15.785 5.690 1.00 42.29 H MOTA 6292 0 **HOH H 328** 85.569 33.598 37.182 1.00 31.78 н ٥ 33.070 -11.287 23.137 1.00 48.90 ATOM 6293 HOH H 329 н ATOM 6294 0 нон н 330 87.593 16.513 19.683 1.00 45.53 H MOTA 6295 0 HOH H 331 116.176 53.631 17.853 1.00 39.81 н 6296 0 HOH H 332 26.940 -11.377 14.930 H MOTA 1.00 39.40 MOTA 6297 O HOH H 333 60.033 28.679 22.456 1.00 32.84 H MOTA 6298 0 HOH H 334 52.472 15.182 2.562 1.00 48.72 н ATOM 6299 ٥ нон н 335 84.377 54.588 4.646 1.00 40.99 н H 0 HOH H 336 115.759 19,970 1.00 46.15 MOTA 6300 67.454 MOTA 6301 0 HOH H 337 88.969 52.684 25.112 1.00 42.31 H 36.351 9.875 1.00 37.11 ATOM 6302 O HOH H 338 12.852 6303 0 нон н 339 97.702 31.578 2.653 1.00 49.82 H ATOM 53.964 26.981 HOH H 340 -6.543 1.00 35.52 H MOTA 6304 0 ATOM 6305 0 HOH H 341 24.475 -17.438 17.094 1.00 38.04 H ATOM 6306 Q HOH H 342 58.530 0.915 19.036 1.00 43.08 Н 6307 0 HOH H 343 77.156 37.203 39.025 1.00 48.54 MOTA Н 6308 0.435 0 HOH H 344 49.978 -1.361 1.00 39.48 ATOM MOTA 6309 0 HOH H 345 53.900 37.104 13.703 1.00 47.74 н 13.575 ATOM 6310 O HOH H 346 77.886 49.625 1.00 57.13 8.721 0.570 1.00 50.38 Н 0 HOH H 347 57.053 6311 ATOM MOTA 6312 0 HOH H 348 96.803 63.745 10.854 1.00 41.14 Н 89.009 70.808 11.906 1.00 45.67 Н ATOM 6313 HOH H 349 MOTA 6314 ٥ HOH H 350 66.363 22.353 8.221 1.00 42.47 Н 52.578 25.044 8.541 1.00 41.16 H ATOM 6315 0 HOH H 351 ATOM 6316 0 HOH H 352 81.789 73.640 -3.536 1.00 50.48 н 0 нон н 353 67.632 -11.181 13.891 1.00 48.24 H MOTA 6317 6318 0 HOH H 354 41.357 -5.652 22,367 1.00 14.47 H ATOM 37.685 -5.096 30.876 1.00 23.96 G MOTA 6319 C1 EDO G 501 38.224 31.883 1.00 23.38 G MOTA 6320 01 EDO G 501 -4.213 MOTA 6321 C2 EDO G 501 38.742 -6.046 30.406 1.00 25.29 G 31.464 1.00 26.30 G MOTA 6322 02 EDO G 501 39.062 -6.931 MOTA 6323 Cl EDO G 502 89.146 26.377 27.000 1.00 41.69 28.343 G 88.631 26.508 1.00 51.10 ATOM 6324 01 **KDO G 502** 6325 C2 EDO G 502 88.436 25.261 26.303 1.00 43.14 G ATOM 88.726 26.967 1.00 41.73 G MOTA 6326 02 EDO G 502 24.052 EDO G 503 85.093 31.920 30.633 1.00 21.00 6327 C1 ATOM G 31,203 1.00 18.65 ATOM 6328 01 EDO G 503 85.283 30.597 6329 EDO G 503 83.846 32.561 31,186 1.00 19.69 ATOM C2 ATOM 6330 02 EDO G 503 84.148 33.101 32.454 1.00 20.94 G 34.956 3.907 25.885 1.00 38.01 EDO G 504 6331 C1 ATOM 1.00 36.69 G 33.976 2.838 25.869 ATOM 6332 01 EDO G 504 ATOM 6333 C2 EDO G 504 36.360 3.344 25.982 1.00 39.84 G ATOM 02 EDO G 504 36.573 2.396 24.935 1.00 33.51 6334 END

Example 4

Binding of altered gluten peptides (peptide analogs) to MHC molecules is assayedwith purified HLA molecules. Binding of labeled peptide to purified HLA DQ2 molecules can be measured as described by Johansen et al. (1996) Int Immmunol (8), 177-82. Briefly, purified DQ2 molecules (50 - 1000 nM) are incubated with the 125-I radiolabeled indicator peptide (MB 65kDa 243-255Y, sequence KPLLIIAEDVEGEY; 20 000 cpm, 1-5 nM) at pH 4.9. After incubation for 24 hours, the peptide bound to DQ2 and the non-bound peptide are separated on Sephadex G25 superfine spun columns. The radioactivity in the bound and non-bound fractions was counted in a gamma-counter, and the fraction of peptide bound to DQ2 (cpm in the bound fraction/total cpm recovered) is calculated. The binding capacities of the peptide binding inhibitors are assayed by testing their ability to inhibit the binding of the labeled indicator peptide. The concentration required to give 50%

inhibition (IC $_{50}$) is calculated. Since the level of IC $_{50}$ may vary between separate titration experiments, the IC $_{50}$ values are compared to the IC $_{50}$ of a reference peptide by determining the relative binding capacity (RBC), which is the ratio: IC $_{50}$ of reference peptide / IC $_{50}$ of test compound. HLA-DQ2 molecules can be isolated by antibody affinity chromatography from lysates of HLA-DQ2 homozygous Epstein Barr virus transformed B-lymphoblastoid cell lines (detergent solubilized) or from water soluble, recombinant molecules produced similarly as described in Example 3 above. The recombinant molecules can be made with or without covalently linked peptide and with a biotin recognition sequence at the C-terminal end of the β -subunit that facilitates adsorption of HLA-DQ2 to several streptavidin coated supports, thereby enabling alternative ways for measurement of IC $_{50}$. A peptide analog with an IC $_{50}$ value of less than 100 μ M is suitable for further screenings.

[92] Alternatively, binding of altered gluten peptides to HLA-DQ2 can also be assayed using the soluble DQ2 heterodimer produced as described in Example 3 above. The presence of the biotin recognition sequence at the C-terminal end of the β-subunit facilitates adsorption of HLA-DQ2 to several streptavidin coated supports, thereby enabling measurement of IC₅₀ or K_I.

Candidate peptide analogs are further tested for their ability to inhibit proliferation of [93] T cells specific for gluten peptides. This is done by using HLA-DQ2 restricted T cell clones (TCC) and glutaraldehyde fixed antigen presenting cells (e.g. Epstein Barr virus transformed B-lymphoid transformed cells) expressing HLA-DQ2. The antigen presenting cells are pelleted and resuspended in RPMI containing 0.05% glutaraldehyde for 90 sec, whereafter glycin to a final concentration of 0.2 M is added for 60 sec. The cells are then washed, counted, and resuspended in PBS or PBS buffered with citrate phosphate to a final pH of 4.9. The fixed APC are incubated overnight with various concentrations of peptides. The inhibitory peptides are usually added 30 min prior to the stimulatory peptide. The antigen presenting cells are then washed twice and resuspended in culture medium of RPMI-1640 supplemented with 15% v/v heat inactivated pooled human serum and the T cells are added. The experiments are performed in triplicates of 3-5 X 10⁴ TCC with 5 X 10⁴ fixed APC and various titrations of inhibitory and stimulatory peptides. Following an incubation period of 48 hours, each culture is pulsed with [3H]-thymidine for an additional 12-18 hours. Cultures are then harvested on fiberglass filters and counted as above. Mean CPM and standard error of the mean are calculated from data determined in triplicate cultures. Peptide analogs that inhibit proliferation to approximately 25% at a concentration of 50 µM or greater are suitable for further screening.

[94] All publications and patent applications cited in this specification are herein incorporated by reference as if each individual publication or patent application were specifically and individually indicated to be incorporated by reference.

[95] Although the foregoing invention has been described in some detail by way of illustration and example for purposes of clarity of understanding, it will be readily apparent to those of ordinary skill in the art in light of the teachings of this invention that certain changes and modifications may be made thereto without departing from the spirit or scope of the appended claims.

WHAT IS CLAIMED IS:

1. An HLA-binding peptide inhibitor; wherein said inhibitor is an analog of an immunogenic gluten oligopeptide of at least about 8 residues in length, wherein the immunogenic gluten oligopeptide is altered by the replacement of one or more amino acids; and wherein said analog binds tightly to HLA molecules; is proteolytically stable; and does not activate disease-specific T cells.

- The HLA-binding peptide inhibitor of Claim 1, wherein said analog comprises
 one or more naturally occurring amino acids, non-naturally occurring amino acids, modified
 amino acids, or amino acid mimetics.
- 3. The HLA-binding peptide inhibitor of Claim 2, wherein said analog is further derivatized to reduce the affinity of the analog for disease-specific T cell receptors.
- 4. The HLA-binding peptide inhibitor of Claim 1, wherein said immunogenic gluten oligopeptides comprises at least one PXP motif.
- 5. The HLA-binding peptide inhibitor of Claim 1, wherein said immunogenic gluten oligopeptides comprises a sequence selected from the group consisting of: PQPELPY; PFPQPELPYP, PQPELPYPQPQLP, PQQSFPEQQPP, VQGQGIIQPEQPAQ, FPEQPQQPYPQQP, FPQQPEQPYPQQP, FSQPEQEFPQPQ; PFPQPQLPY, PQPQLPYPQ, PFPQPELPY; PYPQPELPY and PYPQPQLPY.
- [96] 6. The HLA-binding peptide inhibitor of Claim 1, wherein said inhibitor comprises the sequence PXPQPELPY, where X is Tyr, Trp, Arg, Lys, p-iodo-Phe, 3-iodo-Tyr, p-amino-Phe, 3-amino-Tyr, hydroxylysine, ornithine, Asp or Glu.
 - 7. The HLA-binding peptide inhibitor of Claim 6, wherein said inhibitor is further derivatized to reduce the affinity of the analog for disease-specific T cell receptors.
 - 8. The HLA-binding peptide inhibitor of Claim 6, wherein said inhibitor is further modified to increase binding potency to an MHC molecule.
 - 9. The HLA-binding peptide inhibitor of Claim 1, wherein said inhibitor comprises the sequence $PFPQX_1ELX_2Y$, where X_1 and X_2 are independently selected from 4-hydroxy-Pro, 4-amino-Pro, or 3-hydroxy-Pro, and proline, with the proviso that at least one of X_1 and X_2 is a residue other than proline

10. The HLA-binding peptide inhibitor of Claim 9, wherein said inhibitor is further derivatized to reduce the affinity of the analog for disease-specific T cell receptors.

- 11. The HLA-binding peptide inhibitor of Claim 9, wherein said inhibitor is further modified to increase binding potency to an MHC molecule.
- 12. A method of treating Celiac Sprue and/or dermatitis herpetiformis, the method comprising:

administering to a patient an effective dose of an HLA-binding peptide inhibitor; wherein said HLA-binding peptide inhibitor attenuates gluten toxicity in said patient.

- 13. The method of Claim 12, wherein said HLA-binding peptide inhibitor is administered with a glutenase.
- 14. The method according to Claim 12, wherein said HLA-binding peptide inhibitor is administered orally.
- 15. The method according to Claim 12, wherein said HLA-binding peptide inhibitor is contained in a formulation that comprises an enteric coating.
- 16. A formulation for use in treatment of Celiac Sprue and/or dermatitis herpetiformis, comprising:

an effective dose of an HLA-binding peptide inhibitor and a pharmaceutically acceptable excipient.

- 17. The formulation according to Claim 16, further comprising an enteric coating.
- 18. Use of an HLA-binding peptide inhibitor in the treatment of HLA-DQ2 positive individuals who are either pre-disposed to type I diabetes or have developed symptoms of type I diabetes.
- 19. A computer for producing a three-dimensional representation of a molecule wherein said molecule comprises an HLA-DQ2 molecule bound to an immunogenic gluten oligopeptide, wherein said computer comprises:
- a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises the three-dimensional coordinates of a subset of the atoms in an HLA-DQ2 molecule bound to an immunogenic

gluten oligopeptide;

a working memory for storing instructions for processing said machine-readable data;

- a central-processing unit coupled to said working memory and to said machinereadable data storage medium for processing said machine readable data into said threedimensional representation; and
- a display coupled to said central-processing unit for displaying said three-dimensional representation.
- 20. A computer-assisted method for identifying potential modulators of Celiac Sprue and/or dermatitis herpetiformis, using a programmed computer comprising a processor, a data storage system, an input device, and an output device, comprising the steps of:
- (a) inputting into the programmed computer through said input device data comprising the three-dimensional coordinates of a subset of the atoms in an HLA-DQ2 molecule bound to an immunogenic gluten oligopeptide, thereby generating a criteria data set;
- (b) comparing, using said processor, said criteria data set to a computer database of chemical structures stored in said computer data storage system;
- (c) selecting from said database, using computer methods, chemical structures having a portion that is structurally similar to said criteria data set;
- (d) outputting to said output device the selected chemical structures having a portion similar to said criteria data set.